101801

Access DB# ______

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: SABIHA QAZI Examiner #: 74141 Date: 3/3/06

Art Unit: 1616 Phone Number 30 20622 Serial Number: 09/497,891

Mail Box and Bldg/Room Location: 4C70 4A45 Results Format Preferred (circle): PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need.

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: 16 Hydroxyestrienes as selectively active estrogens

Inventors (please provide full names): Keunzer, Hermann et al.

Earliest Priority Filing Date: 4/27/1999

For Sequence Searches Only Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.

Cls 53 – 65

Please search for the compds 3,16-dihydroxyestra-1,3,5(10)-trienes of formula I in Cl 1

Please note the substituents R^{16} & R^{16}

Specific compds are in Cls 63 & 64

Please see attached sheet

Thank you

STAFF USE ONLY		Type of Search		Vendors and cost where applicable
Searcher	LH	NA Sequence (#)		STN $1244.50
Searcher Phone #:		AA Sequence (#)		Dialog
Searcher Location:		Structure (#)	3	Questel/Orbit
Date Searcher Picked Up:	3/16/06	Bibliographic		Dr.Link
Date Completed:	3/17/06	Litigation		Lexis/Nexis
Searcher Prep & Review Time:	30	Fulltext		Sequence Systems
Clerical Prep Time:	30	Patent Family		WWW/Internet
Online Time:	290	Other		Other (specify)

PTO-1590 (8-01)

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L2            14 S KNAUTHE R?/AU
L3            29 S LESSL M?/AU
L4             2 S L1 AND L2 AND L3
L5            79 S FRITZEMEIER K?/AU
L6            10 S BOEMER U?/AU
L7          3628 S MUELLER G?/AU
L8            21 S KOSEMUND D?/AU
L9             1 S L4 AND L5 AND L6 AND L7 AND L8
L10           70 S HEGELE-HARTUNG C?/AU
L11            1 S L10 AND L9
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L13              SCR 1844
L14              STR
L15          899 SEA FILE=REGISTRY SSS FUL L14 NOT L13
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L16          266 S L12 AND L15
L17           23 S L12 NOT L16

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                 SAV L28 QAZ891A/A
L29          237 S L12 AND L28
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L31         6412 S L15
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L33           24 S L16
L34        46181 S STEROID?/SC,SX
L35          362 S L31 AND L34
L36          316 S L32 AND L34
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L37     2051502 S PHARMA?/SC,SX
L38        1679 S L37 AND L31
L39      652504 S PHARMACEU?/SC,SX
L40         410 S L39 AND L31
L41         404 S L39 AND L32
L42          27 S L35 AND L36 AND L38 AND L40 AND L41
L43          50 S L42 OR L33
L44           1 S L42 AND L33
                E ESTROGEN/CT
L45       93779 S ESTROGEN?
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L47         460 S L15/THU
L48          12 S L42 AND L47
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L14              STR
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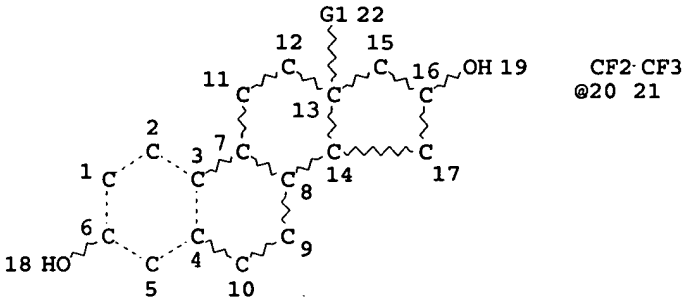

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DEFAULT ECLEVEL IS LIMITED

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RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 22

STEREO ATTRIBUTES: NONE
L15 899 SEA FILE=REGISTRY SSS FUL L14 NOT L13
L16 266 SEA FILE=REGISTRY ABB=ON PLU=ON L12 AND L15
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@20 21	@23 24	@25 26	@27 28	@29 30	@31 32

C~OEt	C~Ak	C~O~Ak	C~CF2 CF3	C~Ak~F
@33 34	@35 36	@37 38 39	@42 41 40	@43 44 45

C~Cy	C~CN	C~Et	C~O~NO2	C~CH2Cl
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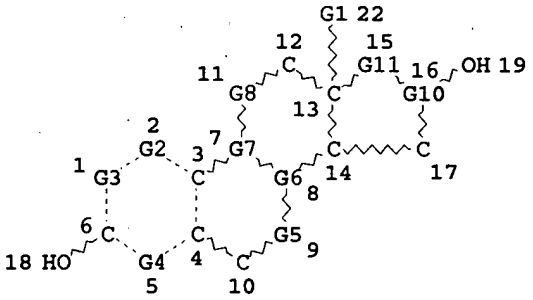
C~G9	C~S~Ak
@58 59	@60 61 63

S @62



C~CH2 CN	C~F
@64 65 66	@67 68

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VAR G6=CH/35/43/48
VAR G7=CH/29/50/25/42
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VAR G9=62/60

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NUMBER OF NODES IS 68

STEREO ATTRIBUTES: NONE
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C~OMe @31 32

C~OEt @33 34
C~Ak @35 36
C~O~Ak @37 38 39
C~CF2 CF3 @42 41 40
C~Ak~F @43 44 45

C~Cy @46 47
C~CN @48 49
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C~G9 @58 59
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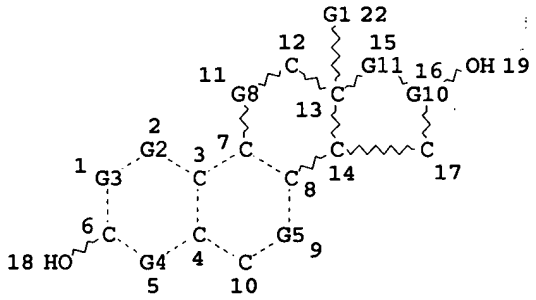

C~CH2 CN @64 65 66
C~F @67 68

VAR G1=ME/ET/CF3/20
VAR G2=CH/23/27/25/29/31/33
VAR G3=CH/23/27/35/37
VAR G4=CH/23/35/25/42/37
VAR G5=CH/23/35/43/37/46
VAR G8=CH2/CH/52/27/58/23/55/35/43/37/46
VAR G9=62/60
VAR G10=CH/35/43/25/42/64
VAR G11=CH2/CH/67/35/43
NODE ATTRIBUTES:
CONNECT IS E2 RC AT 61
CONNECT IS E1 RC AT 62
DEFAULT MLEVEL IS ATOM
GGCAT IS UNS AT 47
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 68

STEREO ATTRIBUTES: NONE
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L33          24 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L16
L34       46181 SEA FILE=HCAPLUS ABB=ON  PLU=ON  STEROID?/SC,SX
L35         362 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L31 AND L34
L36         316 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L32 AND L34
L37     2051502 SEA FILE=HCAPLUS ABB=ON  PLU=ON  PHARMA?/SC,SX
L38        1679 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L37 AND L31
L39      652504 SEA FILE=HCAPLUS ABB=ON  PLU=ON  PHARMACEU?/SC,SX
L40         410 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L39 AND L31
L41         404 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L39 AND L32
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L45       93779 SEA FILE=HCAPLUS ABB=ON  PLU=ON  ESTROGEN?
L46        3741 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L45 AND L31
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L52          24 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L51 AND L33

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L52  ANSWER 1 OF 24  HCAPLUS  COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER:         2000:552017  HCAPLUS
DOCUMENT NUMBER:          133:150782
TITLE:                    synthesis of 16-Hydroxyestratrienes as
                          selectively effective estrogens
INVENTOR(S):              Kuenzer, Hermann; Knauthe, Rudolf; Lessl,
                          Monika; Fritzemeier, Karl-heinrich;
                          Hegele-Hartung, Christa; Boemer, Ulf; Mueller,
                          Gerd; Kosemund, Dirk
PATENT ASSIGNEE(S):       Schering A.-G., Germany
SOURCE:                   Ger. Offen., 34 pp.
                          CODEN: GWXXBX
DOCUMENT TYPE:            Patent
LANGUAGE:                 German
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.           KIND   DATE        APPLICATION NO.        DATE
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     DE 19906159           A1    20000810    DE 1999-19906159
                                                                   1999
                                                                   0209
     CA 2359660            AA    20000817    CA 2000-2359660
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     WO 2000047603         A2    20000817    WO 2000-EP1073
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OTHER SOURCE(S): MARPAT 133:150782

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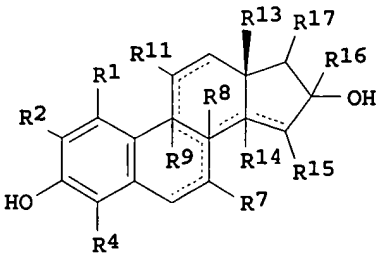

I

AB Synthesis of 16-Hydroxyestratrienes (I) [R1 = halogen, HO, Me, F3C, MeO, EtO, H; R2 = halogen, HO, (un)substituted alkoxy, H; R4 = halogen, fluoroalkyl, F3C, F5C2, (un)substituted alkoxy, H; R7 = halogen, (un)substituted alkyl, (un)substituted alkenyl, (un)substituted alkoxy, (un)substituted heteroaryl, (un)substituted aryl, H; R8 = H, fluoroalkyl, fluoroalkenyl, CN; R9 = H, Me, Et, F3C, F5C2; R11 = NO2O, HO, HS, halogen, chloromethyl, fluoroalkenyl, fluoroalkyl, (un)substituted alkoxy, (un)substituted alkylthio, (un)substituted aryl, (un)substituted heteroaryl, H; R13 = Me, Et, F3C, F5C2; R14 = (un)substituted alkenyl, (un)substituted alkyl, H; R15 = halogen, fluoroalkyl, fluoroalkenyl, =O, =S, SO, SO2, (un)substituted =NH; R14, R15 together = methylene; R16 = fluoroalkyl, fluoroalkenyl, F3C, F5C2,CN, H; R17 = fluoroalkyl, fluoroalkenyl, H, HO] as selectively effective **estrogens** is disclosed. Thus, 16α-estradiol shows a 50% uterine stimulation at 30 υg in in vivo testing.

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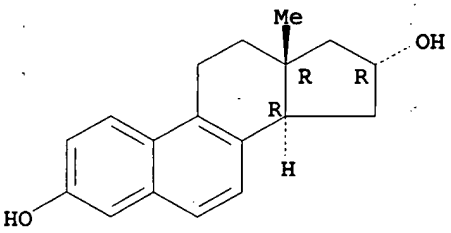
287723-33-5P 287723-35-7P 287723-37-9P
287723-40-4P 287723-41-5P 287723-42-6P
287723-43-7P 287723-44-8P 287723-45-9P
287723-46-0P 287723-47-1P 287723-48-2P
287723-49-3P 287723-50-6P 287723-51-7P
287723-52-8P 287723-53-9P 287723-54-0P
287723-55-1P 287723-56-2P 287723-57-3P
287723-58-4P 287723-59-5P 287723-60-8P
287723-61-9P 287723-62-0P 287723-63-1P
287723-64-2P 287723-65-3P 287723-66-4P
287723-67-5P 287723-68-6P 287723-69-7P
287723-70-0P 287723-71-1P 287723-72-2P
287723-73-3P 287723-75-5P 287723-77-7P
287723-79-9P 287723-80-2P 287723-81-3P
287723-82-4P 287723-83-5P 287723-84-6P
287723-85-7P 287723-86-8P 287723-87-9P
287723-88-0P 287723-89-1P 287723-90-4P
287723-91-5P 287723-92-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis of 16-Hydroxyestratrienes as selectively effective **estrogens**)

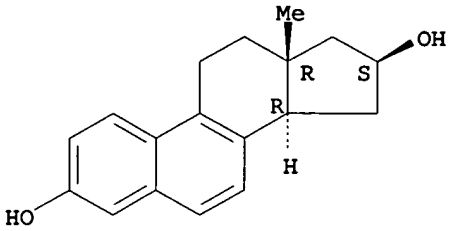
RN 109932-04-9 HCAPLUS
CN Estra-1,3,5(10),6,8-pentaene-3,16-diol, (16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



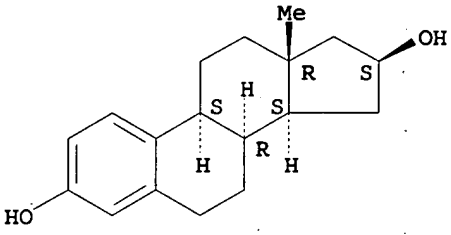
RN 110012-46-9 HCAPLUS
CN Estra-1,3,5(10),6,8-pentaene-3,16-diol, (16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



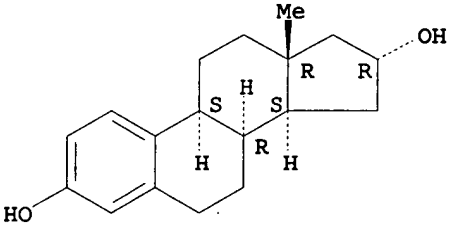
RN 287721-55-5 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, (8α,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



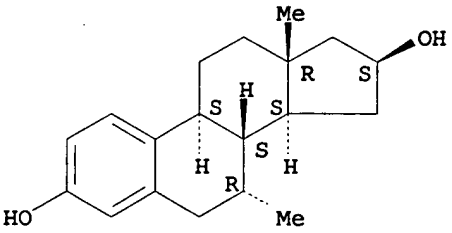
RN 287721-56-6 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, (8α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



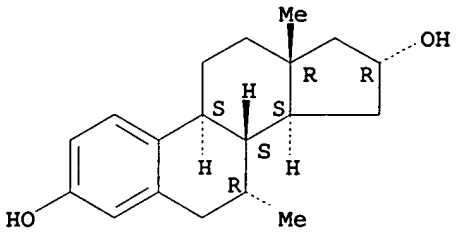
RN 287721-57-7 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 7-methyl-, (7α,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



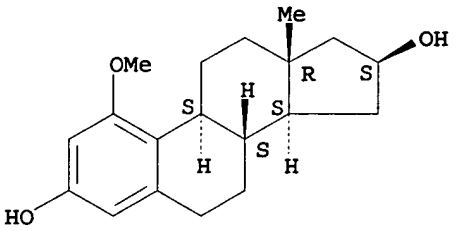
RN 287721-58-8 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 7-methyl-, (7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



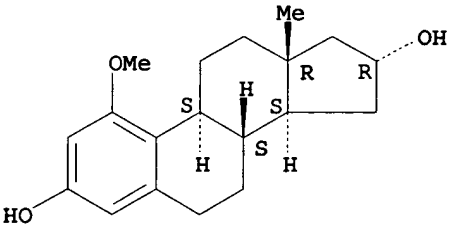
RN 287721-59-9 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 1-methoxy-, (16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



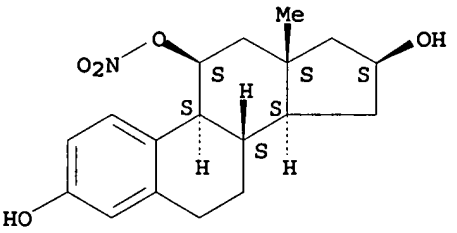
RN 287721-60-2 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 1-methoxy-, (16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 287721-61-3 HCAPLUS
CN Estra-1,3,5(10)-triene-3,11,16-triol, 11-nitrate, (11β,16β)- (9CI) (CA INDEX NAME)

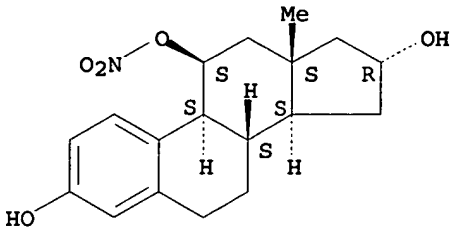
Absolute stereochemistry. Rotation (+).



RN 287721-62-4 HCAPLUS

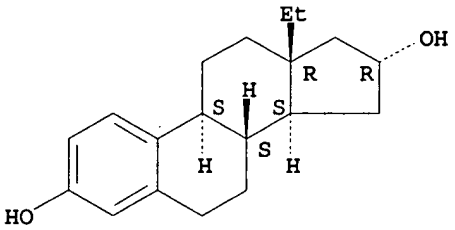
CN Estra-1,3,5(10)-triene-3,11,16-triol, 11-nitrate, (11β,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



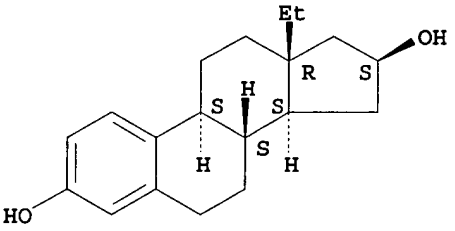
RN 287721-63-5 HCAPLUS
CN Gona-1,3,5(10)-triene-3,16-diol, 13-ethyl-, (16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



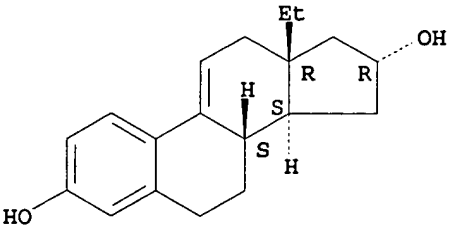
RN 287721-64-6 HCAPLUS
CN Gona-1,3,5(10)-triene-3,16-diol, 13-ethyl-, (16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



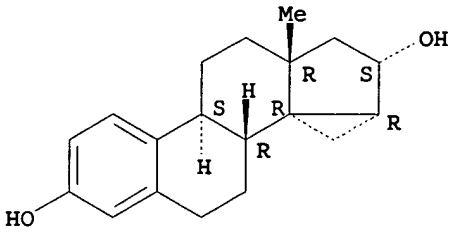
RN 287721-65-7 HCAPLUS
CN Gona-1,3,5(10),9(11)-tetraene-3,16-diol, 13-ethyl-, (16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



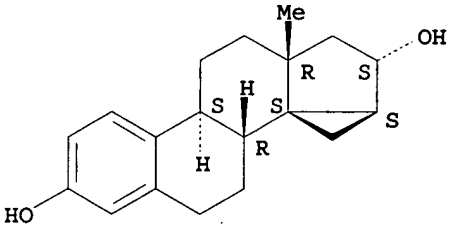
RN 287721-66-8 HCAPLUS
CN Cycloprop[14,15]estra-1,3,5(10)-triene-3,16-diol, 3',15-dihydro-, (14R,15β,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



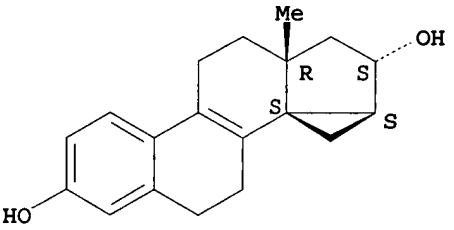
RN 287721-67-9 HCAPLUS
CN Cycloprop[14,15]estra-1,3,5(10)-triene-3,16-diol, 3',15-dihydro-, (14S,15α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



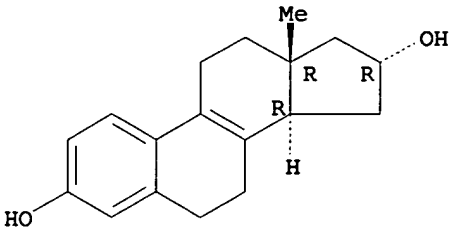
RN 287721-68-0 HCAPLUS
CN Cycloprop[14,15]estra-1,3,5(10),8-tetraene-3,16-diol, 3',15-dihydro-, (14S,15α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



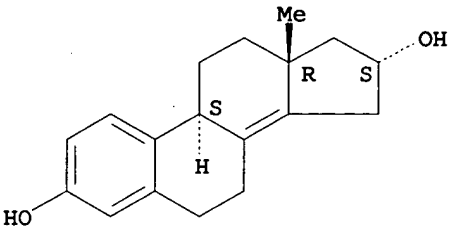
RN 287721-69-1 HCAPLUS
CN Estra-1,3,5(10),8-tetraene-3,16-diol, (16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



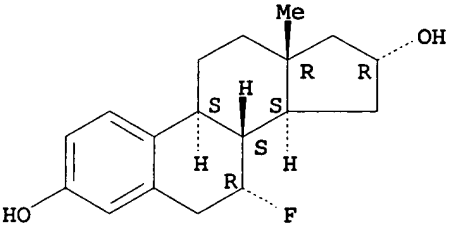
RN 287721-70-4 HCAPLUS
CN Estra-1,3,5(10),8(14)-tetraene-3,16-diol, (16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



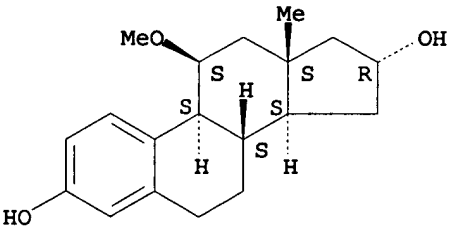
RN 287721-71-5 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 7-fluoro-, (7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



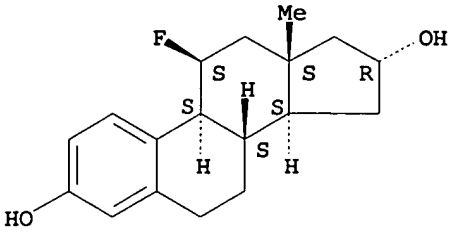
RN 287721-72-6 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-methoxy-, (11β,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



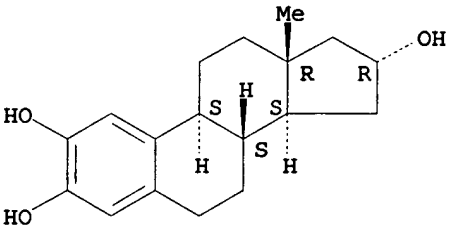
RN 287721-73-7 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-, (11β,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



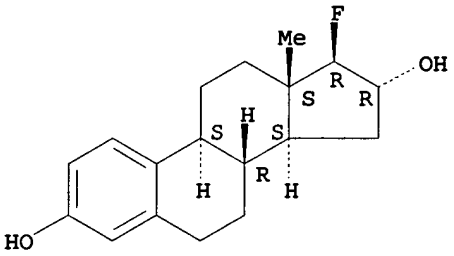
RN 287721-74-8 HCAPLUS
CN Estra-1,3,5(10)-triene-2,3,16-triol, (16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



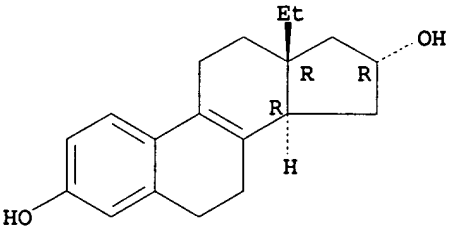
RN 287721-75-9 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 17-fluoro-, (16α,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



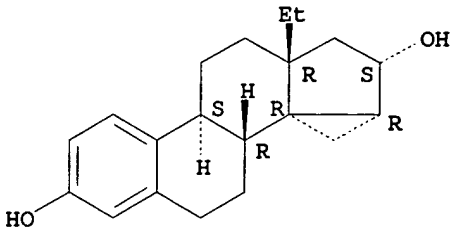
RN 287721-76-0 HCAPLUS
CN Gona-1,3,5(10),8-tetraene-3,16-diol, 13-ethyl-, (16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



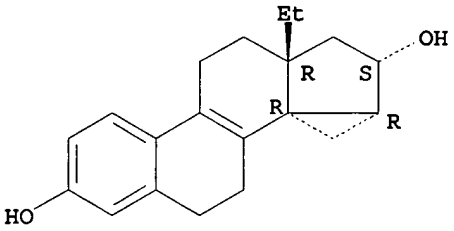
RN 287721-77-1 HCAPLUS
CN Cyclopropa[14,15]gona-1,3,5(10)-triene-3,16-diol, 13-ethyl-3',15-dihydro-, (14R,15β,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



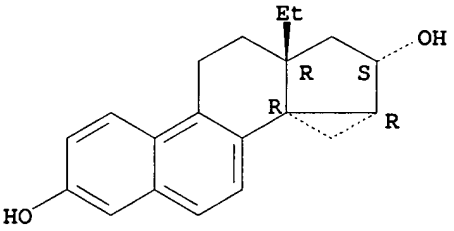
RN 287721-78-2 HCAPLUS
CN Cyclopropa[14,15]gona-1,3,5(10),8-tetraene-3,16-diol, 13-ethyl-3',15-dihydro-, (14R,15β,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



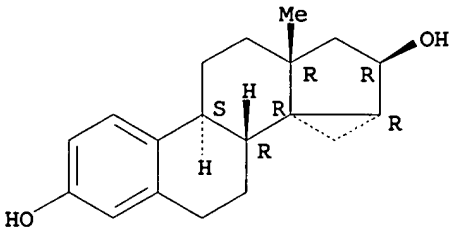
RN 287721-79-3 HCAPLUS
CN Cyclopropa[14,15]gona-1,3,5,7,9-pentaene-3,16-diol, 13-ethyl-3',15-dihydro-, (14R,15β,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



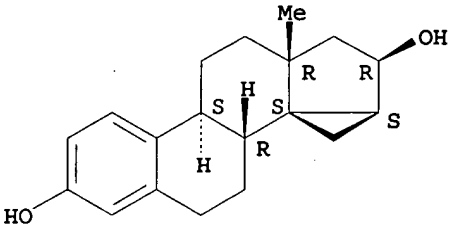
RN 287721-80-6 HCAPLUS
CN Cycloprop[14,15]estra-1,3,5(10)-triene-3,16-diol, 3',15-dihydro-, (14R,15β,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



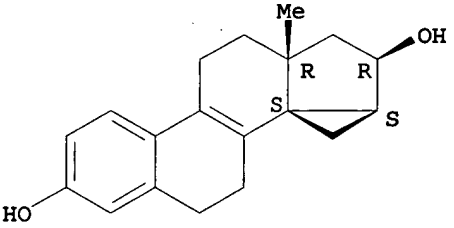
RN 287721-81-7 HCAPLUS
CN Cycloprop[14,15]estra-1,3,5(10)-triene-3,16-diol, 3',15-dihydro-, (14S,15α,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



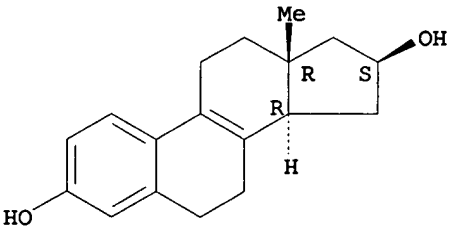
RN 287721-82-8 HCAPLUS
CN Cycloprop[14,15]estra-1,3,5(10),8-tetraene-3,16-diol, 3',15-dihydro-, (14S,15α,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



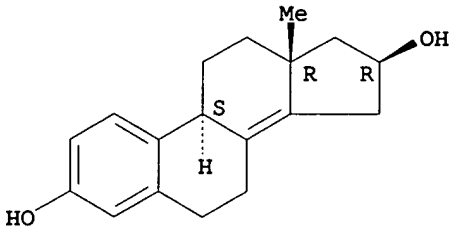
RN 287721-83-9 HCAPLUS
CN Estra-1,3,5(10),8-tetraene-3,16-diol, (16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



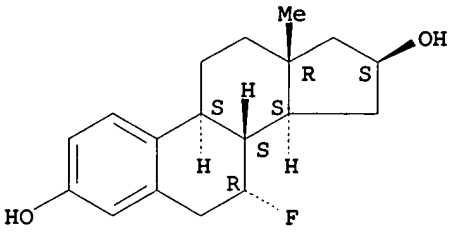
RN 287721-84-0 HCAPLUS
CN Estra-1,3,5(10),8(14)-tetraene-3,16-diol, (16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



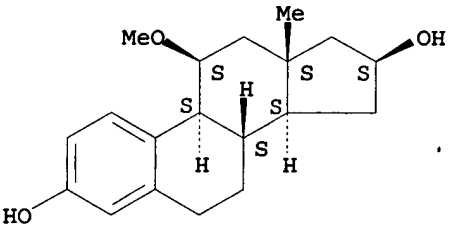
RN 287721-85-1 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 7-fluoro-, (7α,16β)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



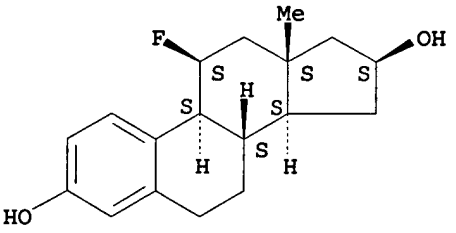
RN 287721-86-2 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-methoxy-,
(11β,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 287721-87-3 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-, (11β,16β)-
(9CI) (CA INDEX NAME)

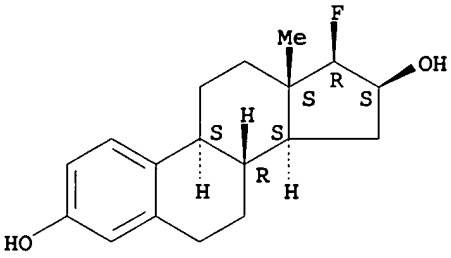
Absolute stereochemistry.



RN 287721-88-4 HCAPLUS

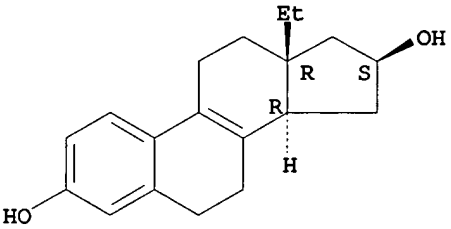
CN Estra-1,3,5(10)-triene-3,16-diol, 17-fluoro-, (16β,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



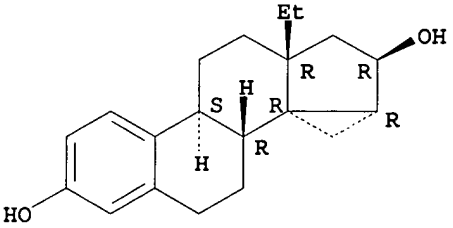
RN 287721-89-5 HCAPLUS
CN Gona-1,3,5(10),8-tetraene-3,16-diol, 13-ethyl-, (16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



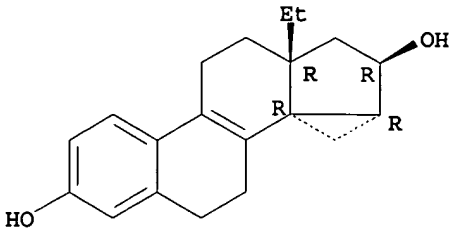
RN 287721-90-8 HCAPLUS
CN Cyclopropa[14,15]gona-1,3,5(10)-triene-3,16-diol, 13-ethyl-3',15-dihydro-, (14R,15β,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



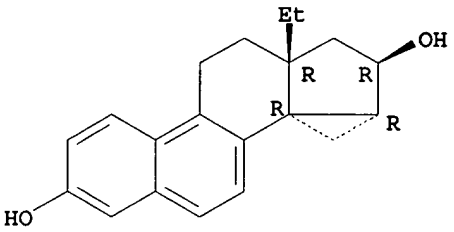
RN 287721-91-9 HCAPLUS
CN Cyclopropa[14,15]gona-1,3,5(10),8-tetraene-3,16-diol, 13-ethyl-3',15-dihydro-, (14R,15β,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



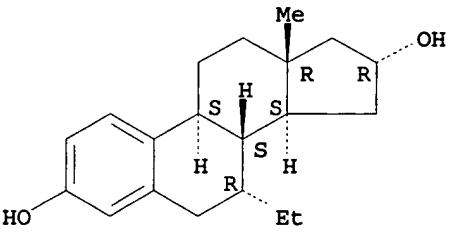
RN 287721-92-0 HCAPLUS
CN Cyclopropa[14,15]gona-1,3,5,7,9-pentaene-3,16-diol, 13-ethyl-3',15-dihydro-, (14R,15β,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



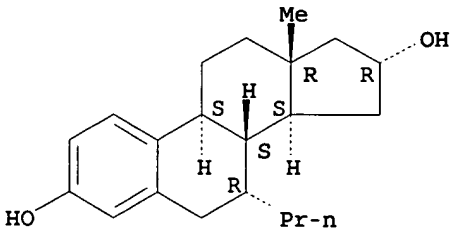
RN 287721-93-1 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 7-ethyl-, (7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 287721-94-2 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 7-propyl-, (7α,16α)- (9CI) (CA INDEX NAME)

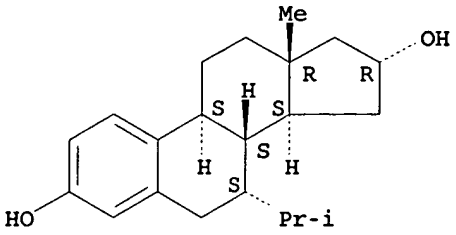
Absolute stereochemistry.



RN 287721-95-3 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 7-(1-methylethyl)-,

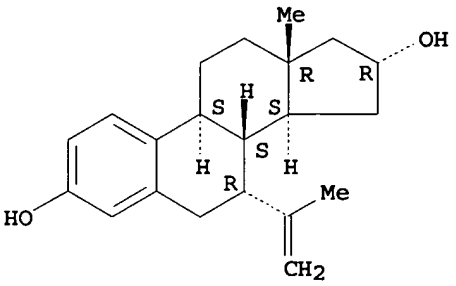
(7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



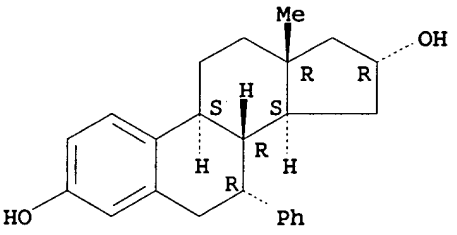
RN 287721-96-4 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 7-(1-methylethenyl)-, (7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



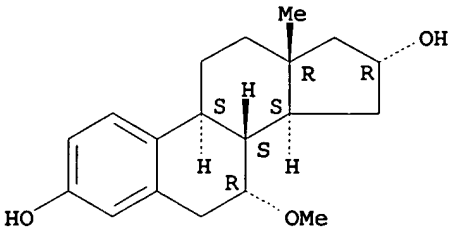
RN 287721-97-5 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 7-phenyl-, (7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



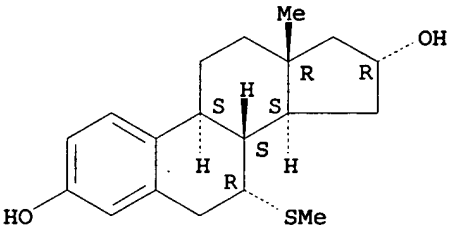
RN 287721-98-6 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 7-methoxy-, (7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



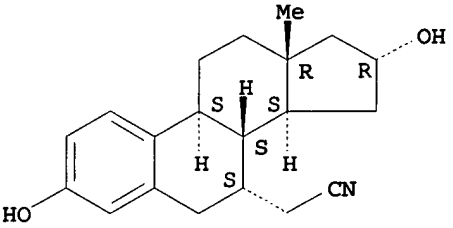
RN 287721-99-7 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 7-(methylthio)-, (7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



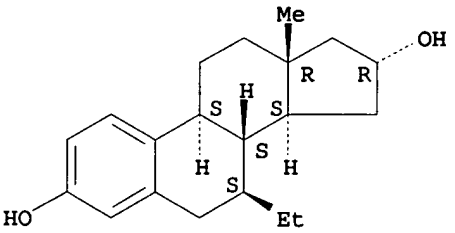
RN 287722-00-3 HCAPLUS
CN Estra-1,3,5(10)-triene-7-acetonitrile, 3,16-dihydroxy-, (7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



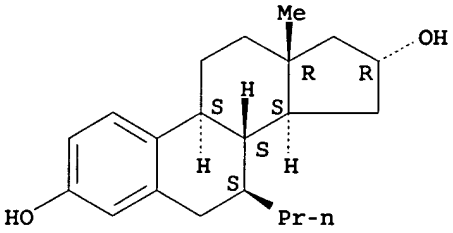
RN 287722-01-4 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 7-ethyl-, (7β,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



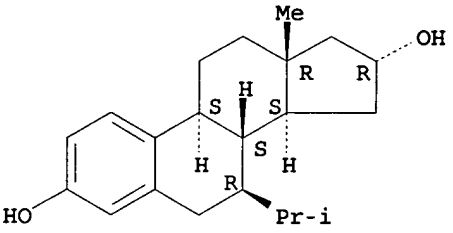
RN 287722-02-5 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 7-propyl-, (7β,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



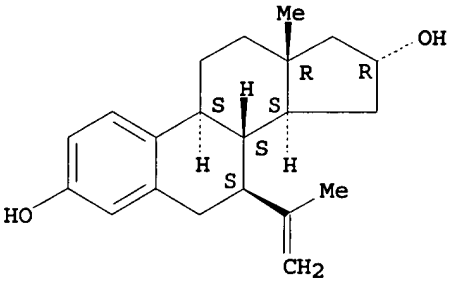
RN 287722-03-6 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 7-(1-methylethyl)-, (7β,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



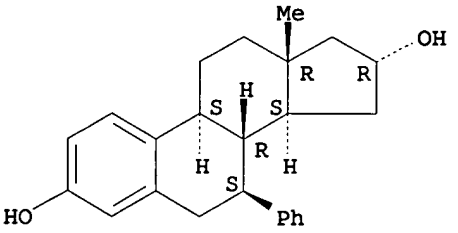
RN 287722-04-7 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 7-(1-methylethenyl)-, (7β,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



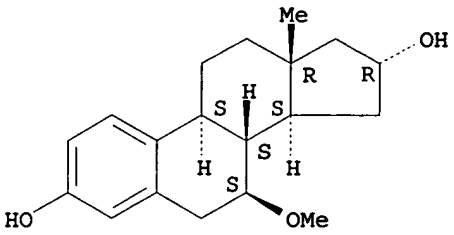
RN 287722-05-8 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 7-phenyl-, (7β,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



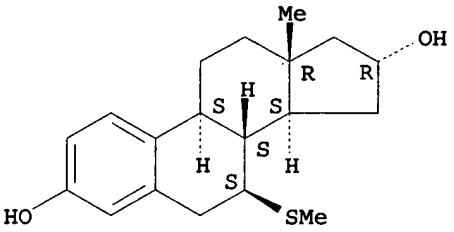
RN 287722-06-9 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 7-methoxy-, (7β,16α)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



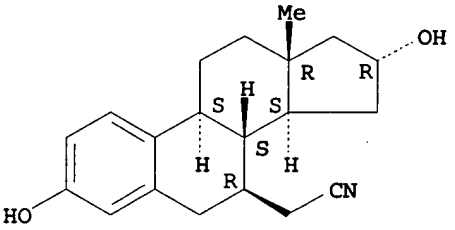
RN 287722-07-0 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 7-(methylthio)-,
(7β,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



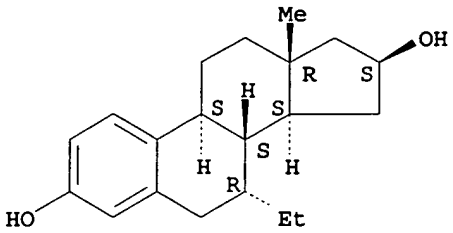
RN 287722-08-1 HCAPLUS
CN Estra-1,3,5(10)-triene-7-acetonitrile, 3,16-dihydroxy-,
(7β,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



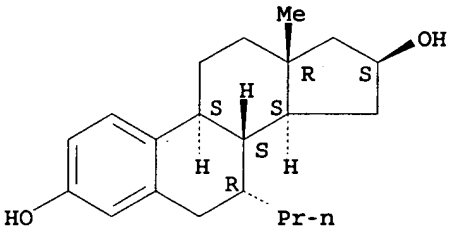
RN 287722-09-2 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 7-ethyl-, (7α,16β)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



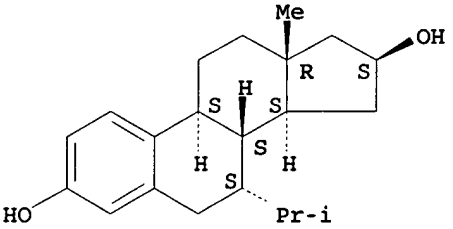
RN 287722-10-5 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 7-propyl-, (7α,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



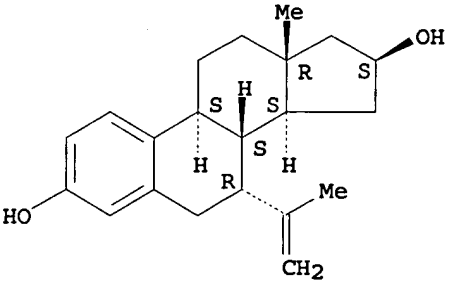
RN 287722-11-6 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 7-(1-methylethyl)-, (7α,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 287722-12-7 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 7-(1-methylethenyl)-, (7α,16β)- (9CI) (CA INDEX NAME)

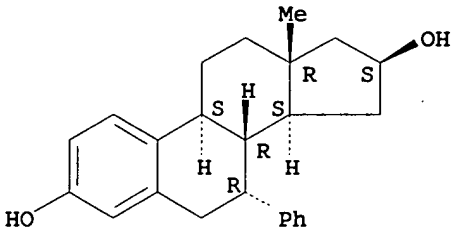
Absolute stereochemistry.



RN 287722-13-8 HCAPLUS

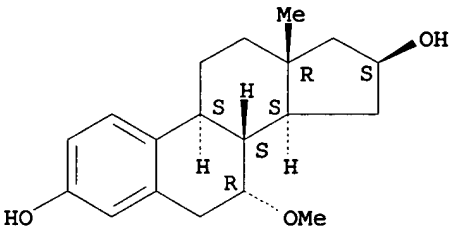
CN Estra-1,3,5(10)-triene-3,16-diol, 7-phenyl-, (7α,16β)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



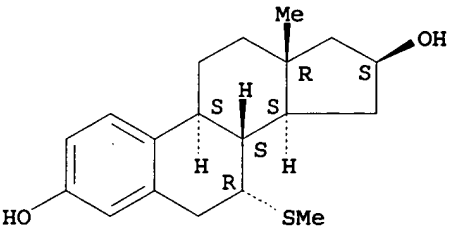
RN 287722-14-9 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 7-methoxy-, (7α,16β)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



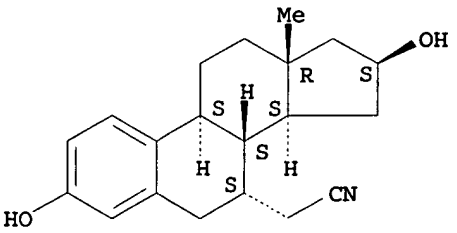
RN 287722-15-0 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 7-(methylthio)-,
(7α,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



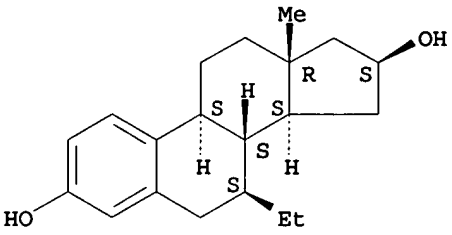
RN 287722-16-1 HCAPLUS
CN Estra-1,3,5(10)-triene-7-acetonitrile, 3,16-dihydroxy-,
(7α,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



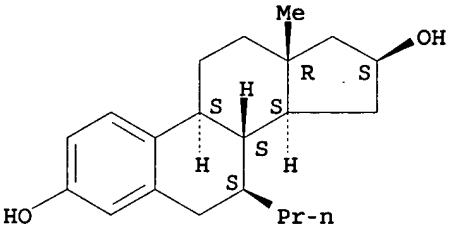
RN 287722-17-2 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 7-ethyl-, (7β,16β)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



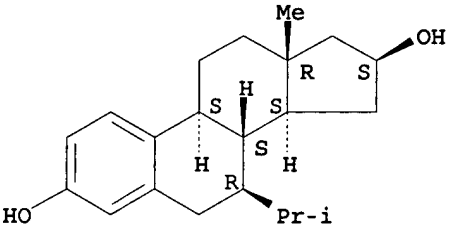
RN 287722-18-3 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 7-propyl-, (7β,16β)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



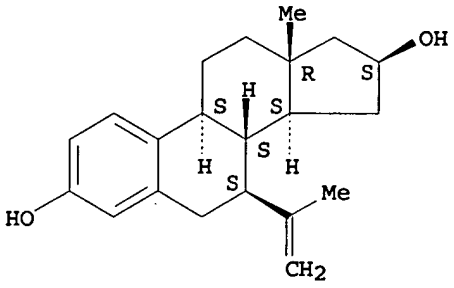
RN 287722-19-4 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 7-(1-methylethyl)-,
(7β,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



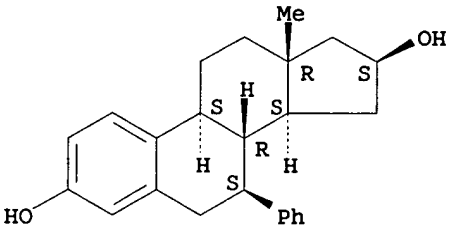
RN 287722-20-7 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 7-(1-methylethenyl)-,
(7β,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



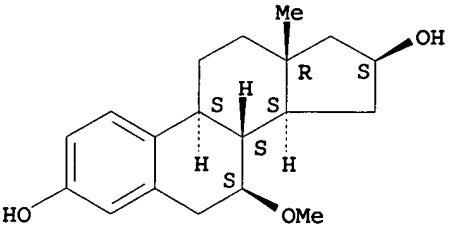
RN 287722-21-8 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 7-phenyl-, (7β,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



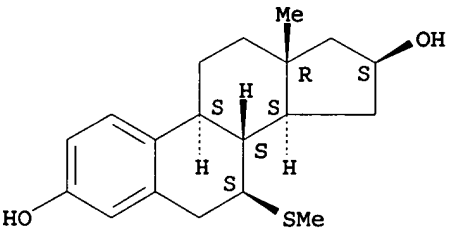
RN 287722-22-9 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 7-methoxy-, (7β,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 287722-23-0 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 7-(methylthio)-, (7β,16β)- (9CI) (CA INDEX NAME)

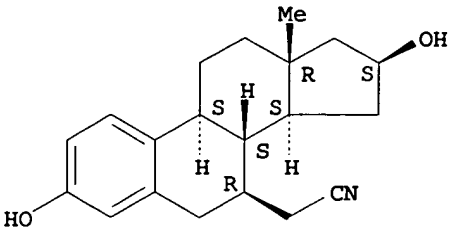
Absolute stereochemistry.



RN 287722-24-1 HCAPLUS

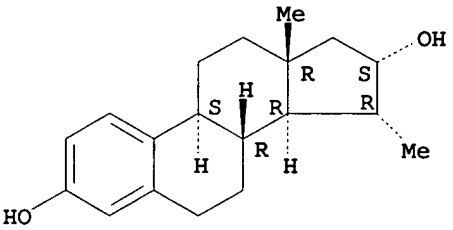
CN Estra-1,3,5(10)-triene-7-acetonitrile, 3,16-dihydroxy-, (7β,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



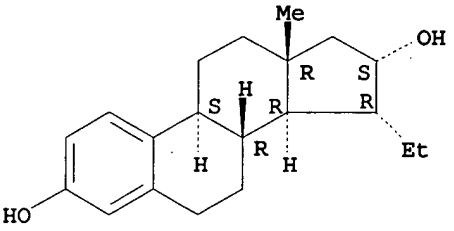
RN 287722-25-2 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 15-methyl-, (15α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



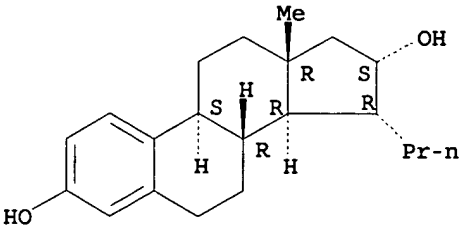
RN 287722-26-3 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 15-ethyl-, (15α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



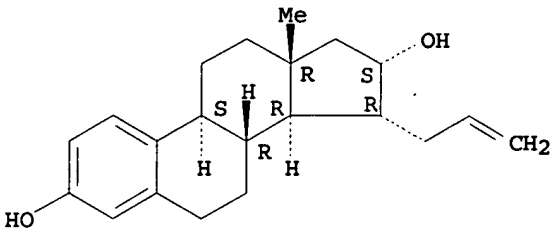
RN 287722-27-4 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 15-propyl-, (15α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



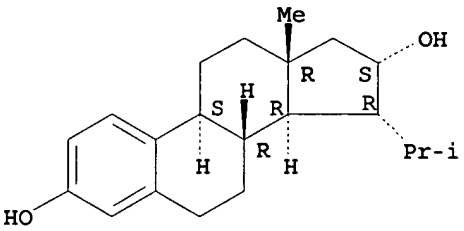
RN 287722-28-5 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 15-(2-propenyl)-, (15α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



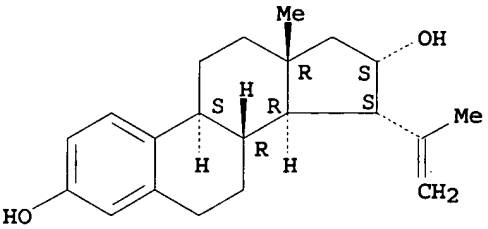
RN 287722-29-6 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 15-(1-methylethyl)-, (15α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



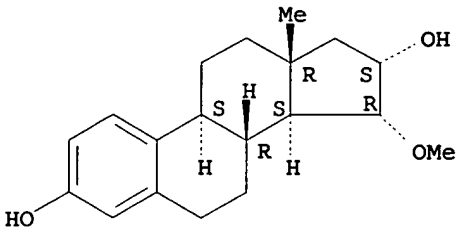
RN 287722-30-9 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 15-(1-methylethenyl)-, (15α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



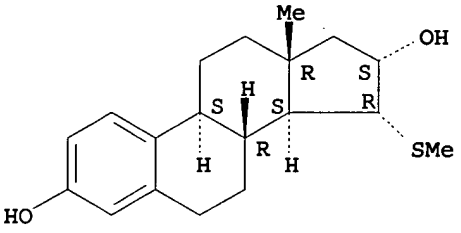
RN 287722-31-0 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 15-methoxy-, (15α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



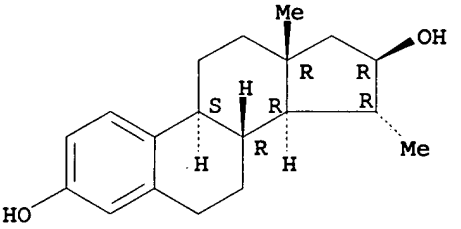
RN 287722-32-1 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 15-(methylthio)-, (15α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



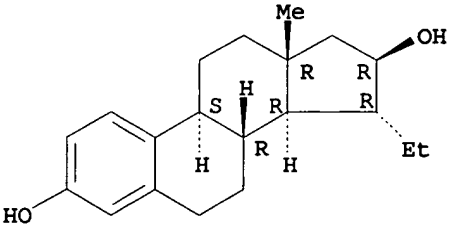
RN 287722-33-2 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 15-methyl-, (15α,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



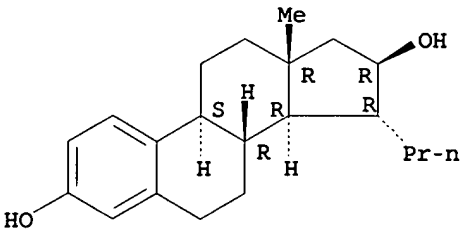
RN 287722-34-3 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 15-ethyl-, (15α,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



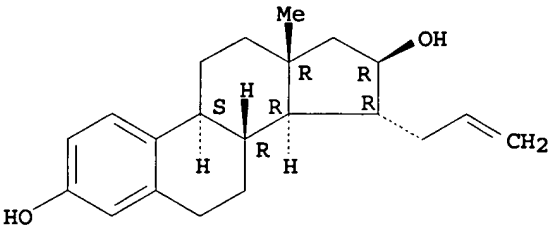
RN 287722-35-4 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 15-propyl-, (15α,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



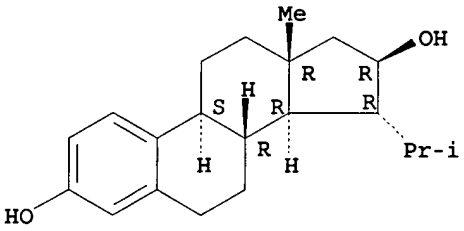
RN 287722-36-5 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 15-(2-propenyl)-, (15α,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



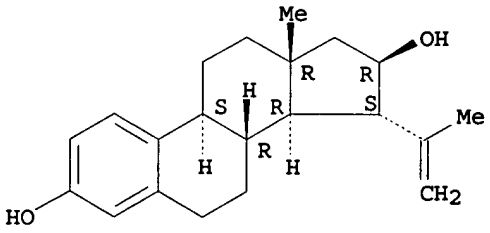
RN 287722-37-6 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 15-(1-methylethyl)-, (15α,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 287722-38-7 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 15-(1-methylethenyl)-, (15α,16β)- (9CI) (CA INDEX NAME)

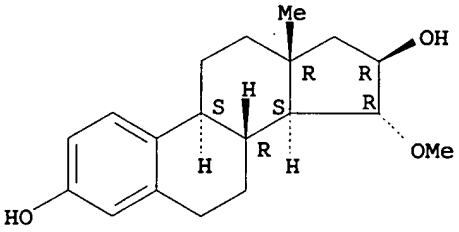
Absolute stereochemistry.



RN 287722-39-8 HCAPLUS

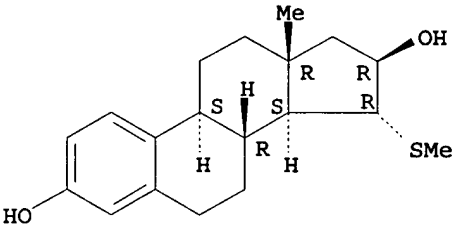
CN Estra-1,3,5(10)-triene-3,16-diol, 15-methoxy-, (15α,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



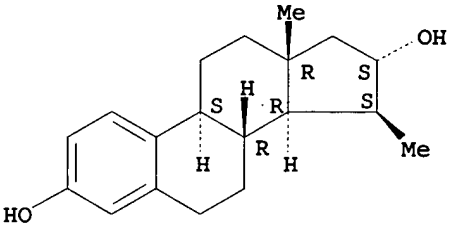
RN 287722-40-1 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 15-(methylthio)-, (15α,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



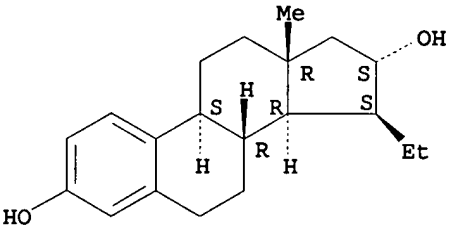
RN 287722-41-2 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 15-methyl-, (15β,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



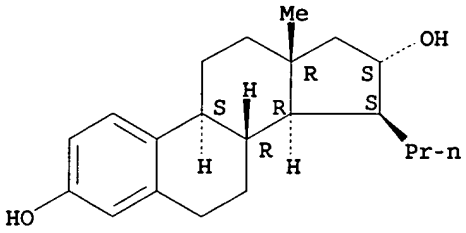
RN 287722-42-3 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 15-ethyl-, (15β,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



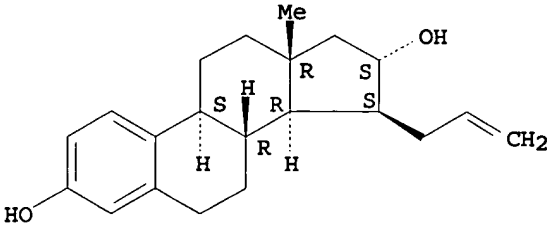
RN 287722-43-4 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 15-propyl-, (15β,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



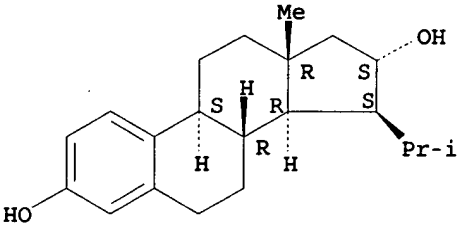
RN 287722-44-5 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 15-(2-propenyl)-, (15β,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



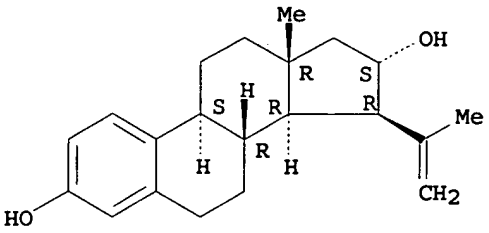
RN 287722-45-6 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 15-(1-methylethyl)-, (15β,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



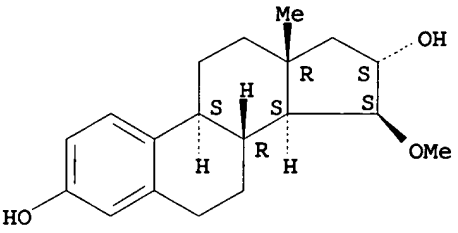
RN 287722-46-7 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 15-(1-methylethenyl)-, (15β,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



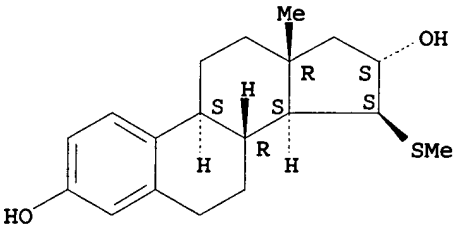
RN 287722-47-8 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 15-methoxy-, (15β,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



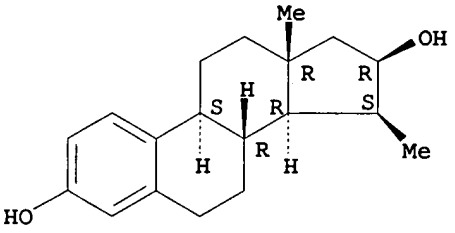
RN 287722-48-9 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 15-(methylthio)-, (15β,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



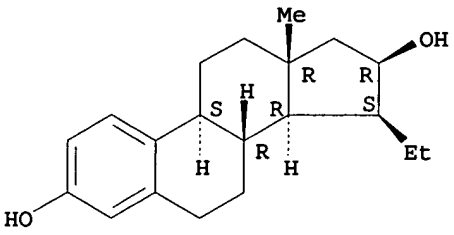
RN 287722-49-0 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 15-methyl-, (15β,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



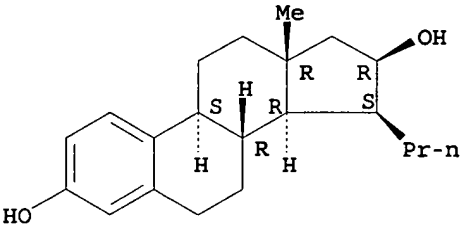
RN 287722-50-3 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 15-ethyl-, (15β,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



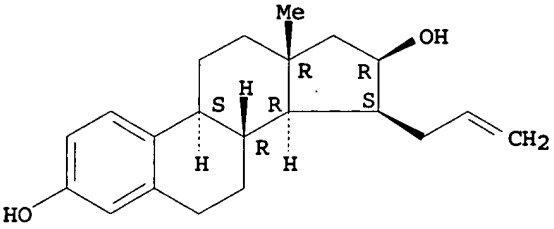
RN 287722-51-4 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 15-propyl-, (15β,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



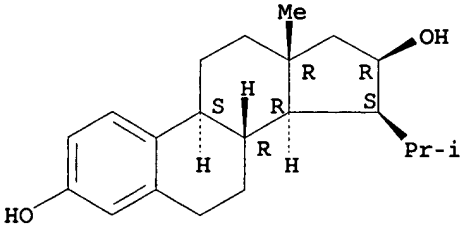
RN 287722-52-5 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 15-(2-propenyl)-, (15β,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 287722-53-6 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 15-(1-methylethyl)-, (15β,16β)- (9CI) (CA INDEX NAME)

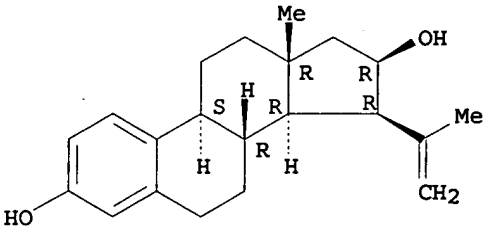
Absolute stereochemistry.



RN 287722-54-7 HCAPLUS

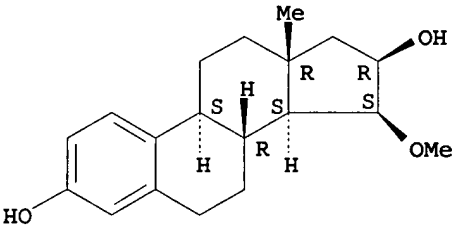
CN Estra-1,3,5(10)-triene-3,16-diol, 15-(1-methylethenyl)-, (15β,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



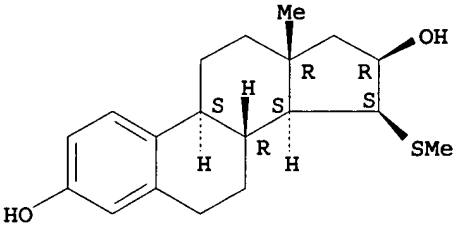
RN 287722-55-8 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 15-methoxy-, (15β,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



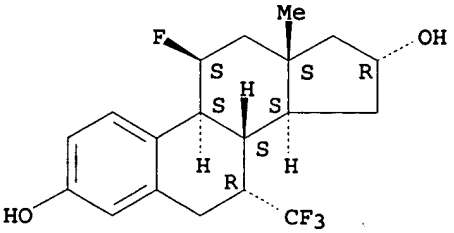
RN 287722-56-9 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 15-(methylthio)-, (15β,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



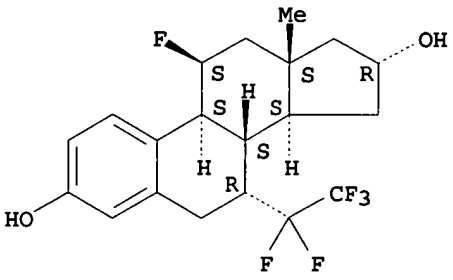
RN 287722-57-0 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-(trifluoromethyl)-, (7α,11β,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



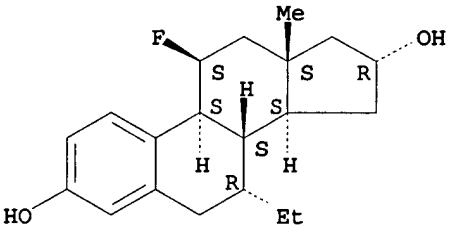
RN 287722-58-1 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-(pentafluoroethyl)-, (7α,11β,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



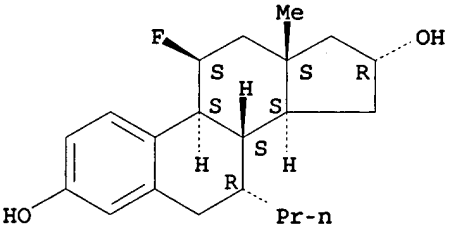
RN 287722-59-2 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 7-ethyl-11-fluoro-, (7α,11β,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



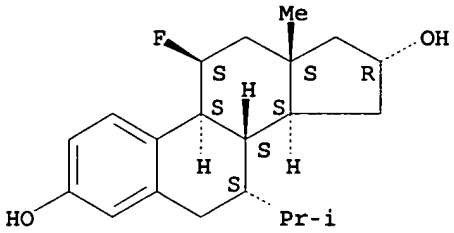
RN 287722-60-5 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-propyl-, (7α,11β,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



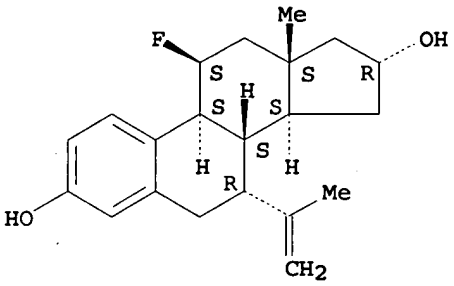
RN 287722-61-6 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-(1-methylethyl)-, (7α,11β,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



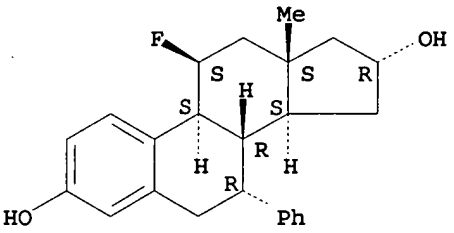
RN 287722-62-7 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-(1-methylethenyl)-, (7α,11β,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



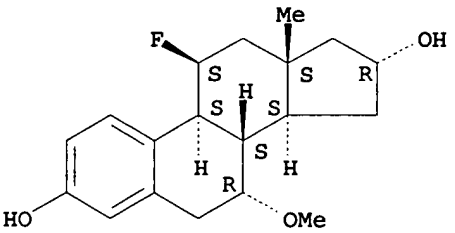
RN 287722-63-8 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-phenyl-, (7α,11β,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 287722-64-9 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-methoxy-, (7α,11β,16α)- (9CI) (CA INDEX NAME)

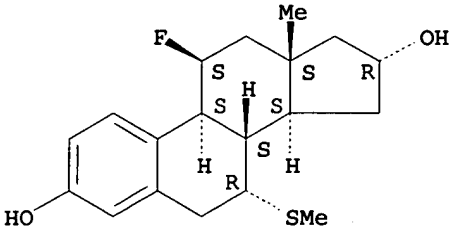
Absolute stereochemistry.



RN 287722-65-0 HCAPLUS

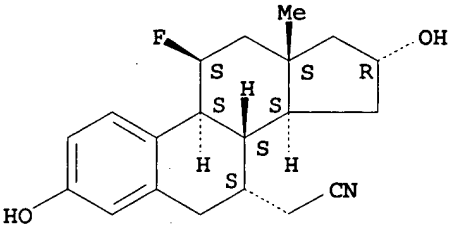
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-(methylthio)-, (7α,11β,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



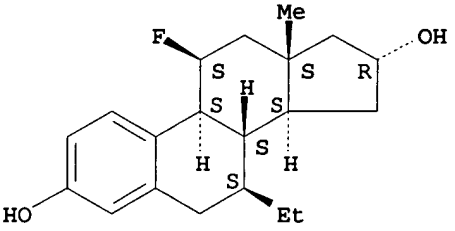
RN 287722-66-1 HCAPLUS
CN Estra-1,3,5(10)-triene-7-acetonitrile, 11-fluoro-3,16-dihydroxy-, (7α,11β,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



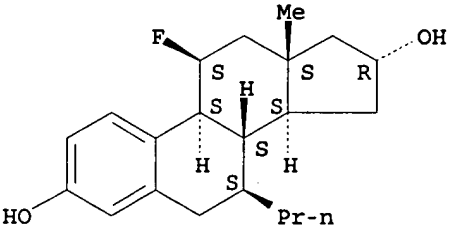
RN 287722-67-2 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 7-ethyl-11-fluoro-, (7β,11β,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



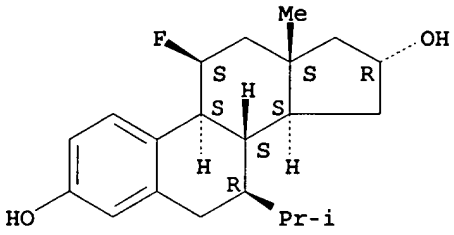
RN 287722-68-3 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-propyl-, (7β,11β,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



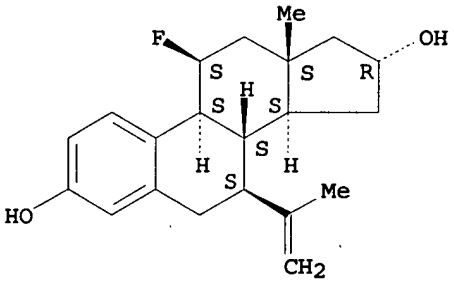
RN 287722-69-4 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-(1-methylethyl)-, (7β,11β,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



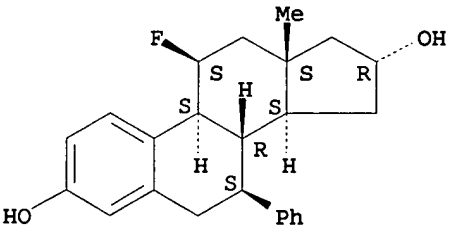
RN 287722-70-7 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-(1-methylethenyl)-, (7β,11β,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



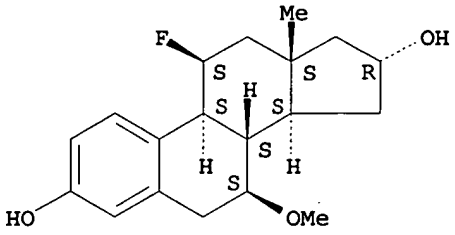
RN 287722-71-8 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-phenyl-, (7β,11β,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



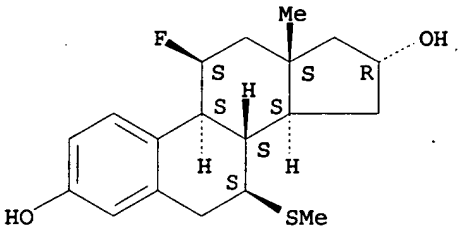
RN 287722-72-9 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-methoxy-, (7β,11β,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



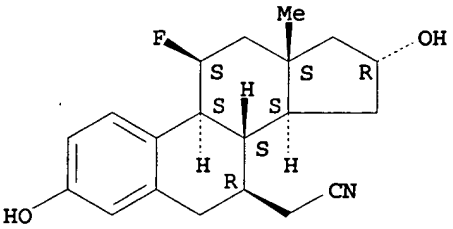
RN 287722-73-0 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-(methylthio)-, (7β,11β,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



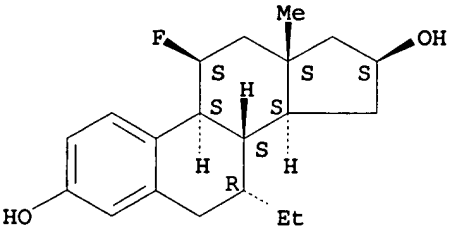
RN 287722-74-1 HCAPLUS
CN Estra-1,3,5(10)-triene-7-acetonitrile, 11-fluoro-3,16-dihydroxy-, (7β,11β,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



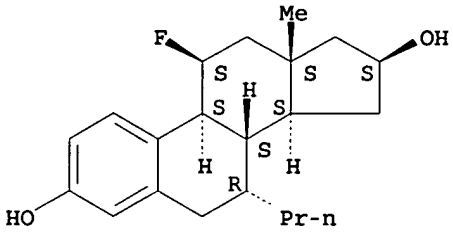
RN 287722-75-2 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 7-ethyl-11-fluoro-, (7α,11β,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



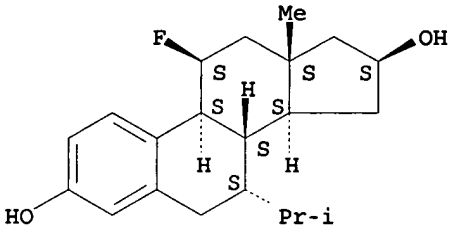
RN 287722-76-3 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-propyl-, (7α,11β,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



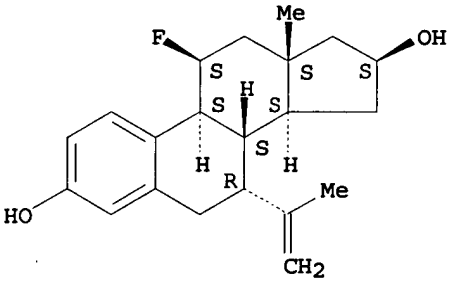
RN 287722-77-4 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-(1-methylethyl)-, (7α,11β,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



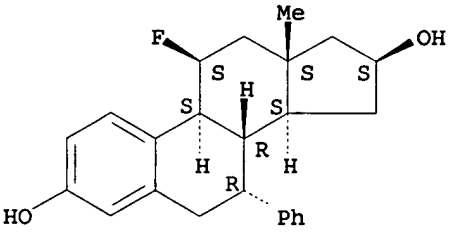
RN 287722-78-5 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-(1-methylethenyl)-, (7α,11β,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



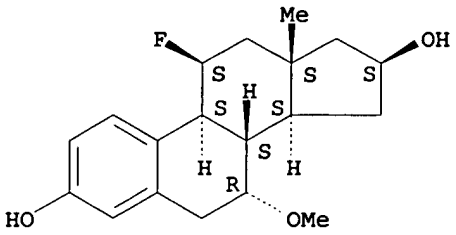
RN 287722-79-6 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-phenyl-, (7α,11β,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



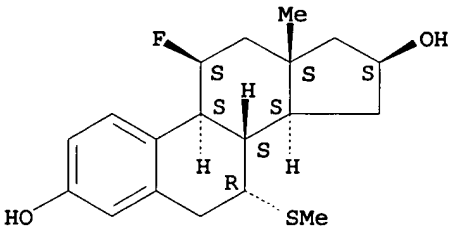
RN 287722-80-9 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-methoxy-, (7α,11β,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



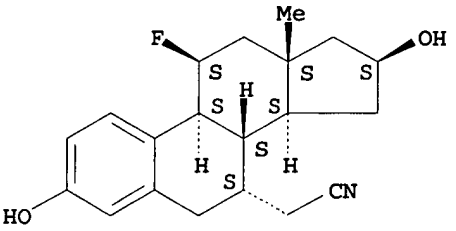
RN 287722-81-0 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-(methylthio)-, (7α,11β,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



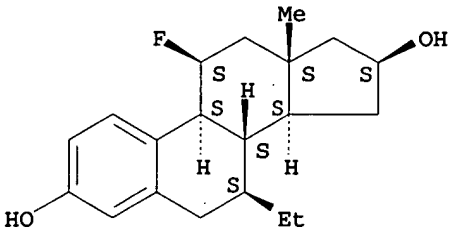
RN 287722-82-1 HCAPLUS
CN Estra-1,3,5(10)-triene-7-acetonitrile, 11-fluoro-3,16-dihydroxy-, (7α,11β,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



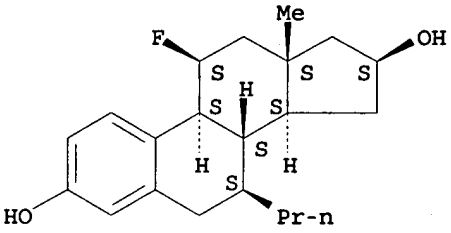
RN 287722-83-2 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 7-ethyl-11-fluoro-, (7β,11β,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



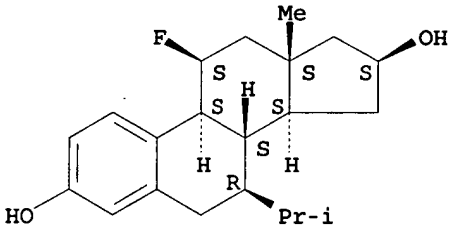
RN 287722-84-3 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-propyl-, (7β,11β,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



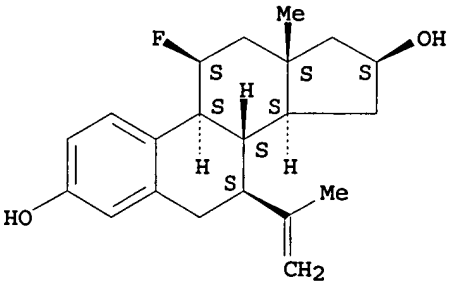
RN 287722-85-4 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-(1-methylethyl)-, (7β,11β,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 287722-86-5 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-(1-methylethenyl)-, (7β,11β,16β)- (9CI) (CA INDEX NAME)

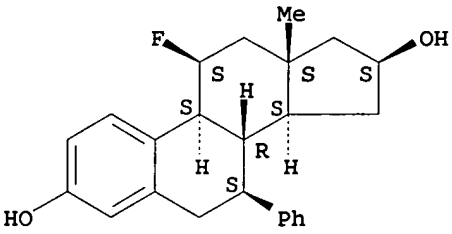
Absolute stereochemistry.



RN 287722-87-6 HCAPLUS

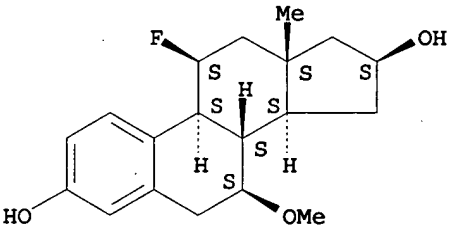
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-phenyl-, (7β,11β,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



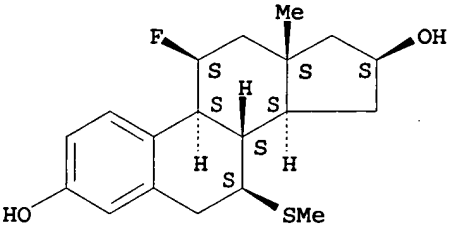
RN 287722-88-7 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-methoxy-, (7β,11β,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



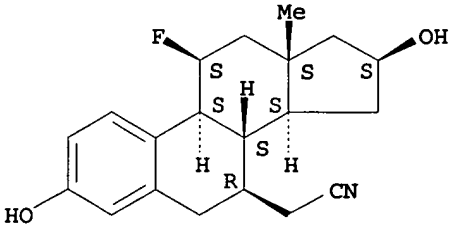
RN 287722-89-8 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-(methylthio)-, (7β,11β,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



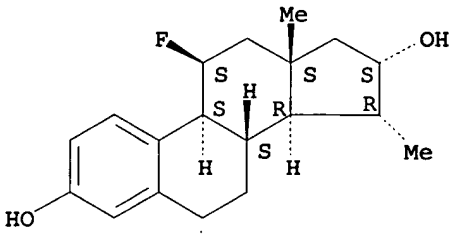
RN 287722-90-1 HCAPLUS
CN Estra-1,3,5(10)-triene-7-acetonitrile, 11-fluoro-3,16-dihydroxy-, (7β,11β,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



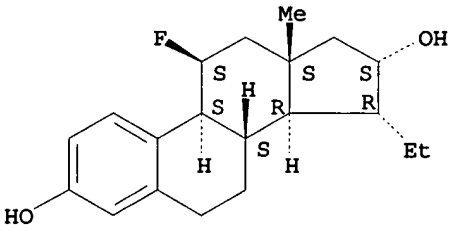
RN 287722-91-2 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-methyl-, (11β,15α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



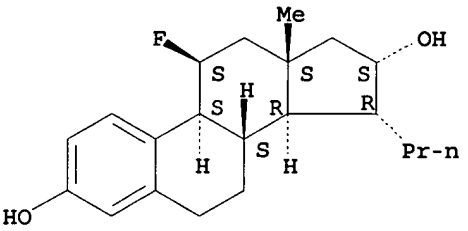
RN 287722-92-3 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 15-ethyl-11-fluoro-, (11β,15α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



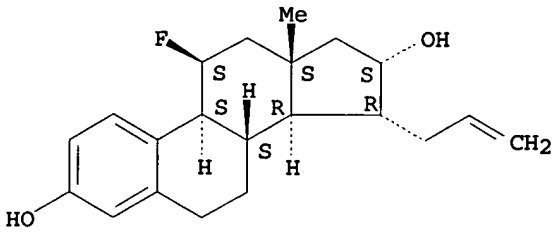
RN 287722-93-4 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-propyl-, (11β,15α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



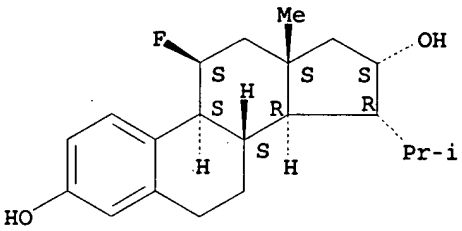
RN 287722-94-5 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(2-propenyl)-, (11β,15α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



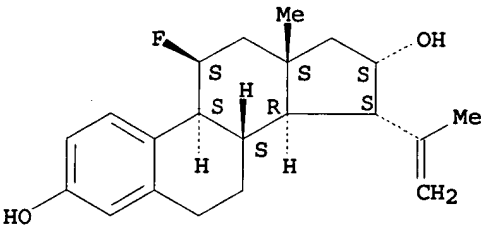
RN 287722-95-6 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(1-methylethyl)-, (11β,15α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



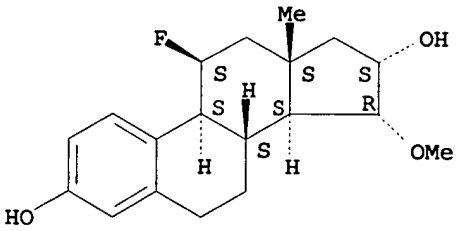
RN 287722-96-7 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(1-methylethenyl)-, (11β,15α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



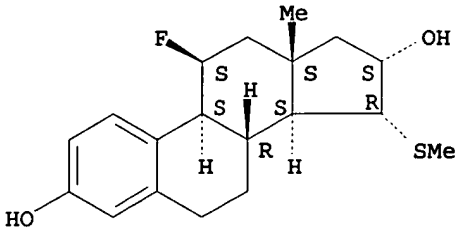
RN 287722-97-8 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-methoxy-, (11β,15α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



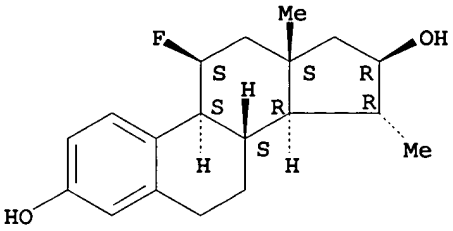
RN 287722-98-9 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(methylthio)-, (11β,15α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



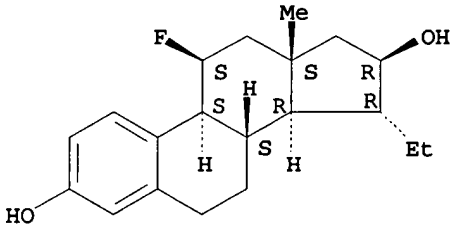
RN 287722-99-0 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-methyl-, (11β,15α,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



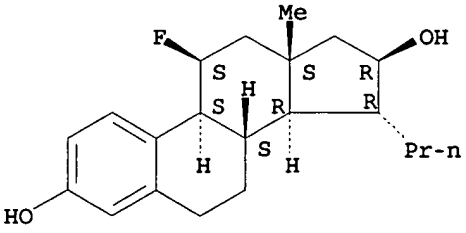
RN 287723-00-6 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 15-ethyl-11-fluoro-, (11β,15α,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 287723-01-7 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-propyl-, (11β,15α,16β)- (9CI) (CA INDEX NAME)

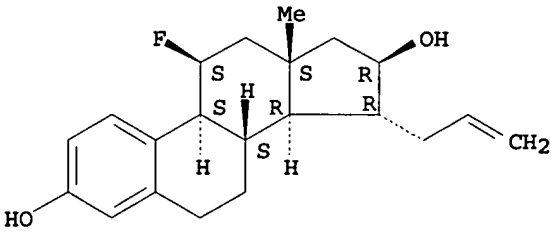
Absolute stereochemistry.



RN 287723-02-8 HCAPLUS

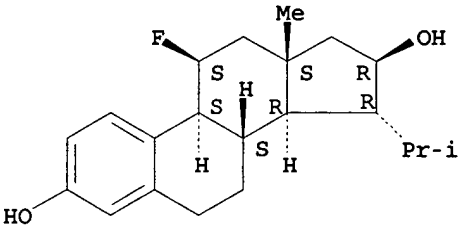
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(2-propenyl)-, (11β,15α,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



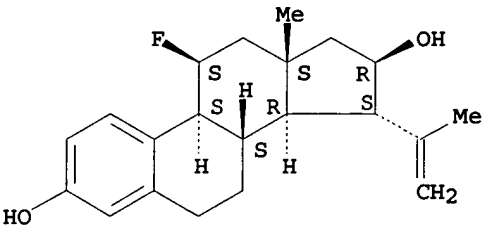
RN 287723-03-9 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(1-methylethyl)-, (11β,15α,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



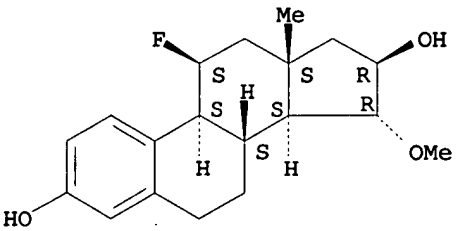
RN 287723-04-0 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(1-methylethenyl)-, (11β,15α,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



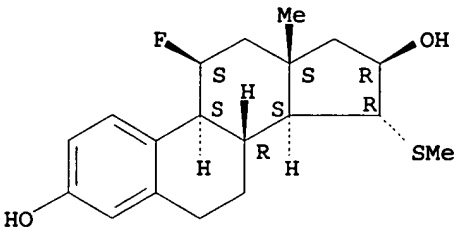
RN 287723-05-1 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-methoxy-, (11β,15α,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



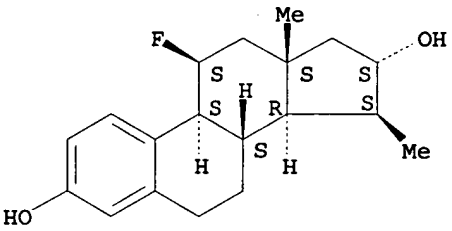
RN 287723-06-2 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(methylthio)-, (11β,15α,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



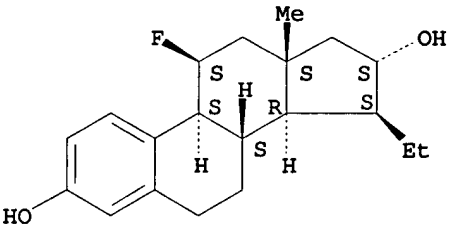
RN 287723-07-3 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-methyl-, (11β,15β,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



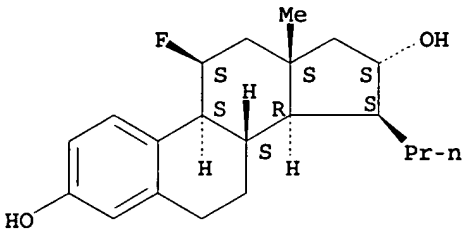
RN 287723-08-4 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 15-ethyl-11-fluoro-, (11β,15β,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



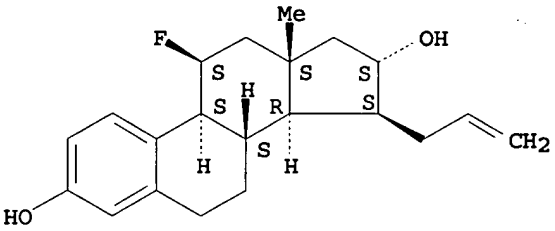
RN 287723-09-5 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-propyl-, (11β,15β,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



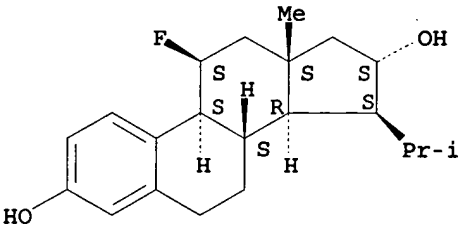
RN 287723-10-8 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(2-propenyl)-, (11β,15β,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



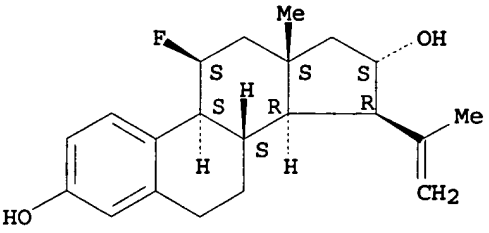
RN 287723-11-9 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(1-methylethyl)-, (11β,15β,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



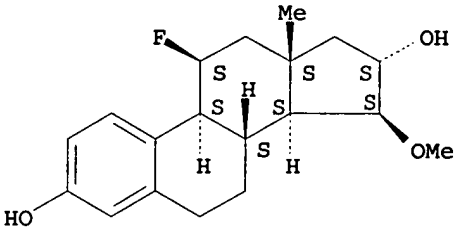
RN 287723-12-0 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(1-methylethenyl)-, (11β,15β,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



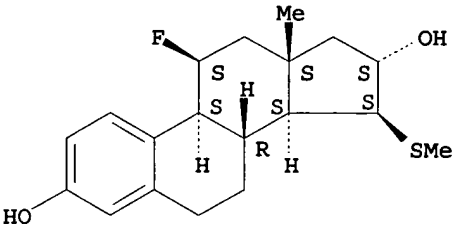
RN 287723-13-1 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-methoxy-, (11β,15β,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



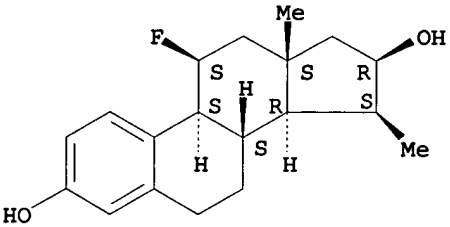
RN 287723-14-2 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(methylthio)-, (11β,15β,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



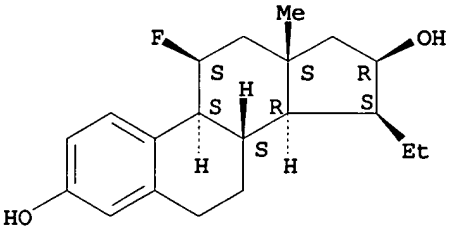
RN 287723-15-3 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-methyl-, (11β,15β,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 287723-16-4 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 15-ethyl-11-fluoro-, (11β,15β,16β)- (9CI) (CA INDEX NAME)

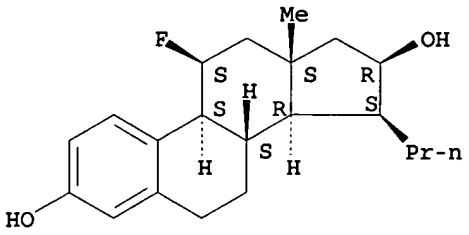
Absolute stereochemistry.



RN 287723-17-5 HCAPLUS

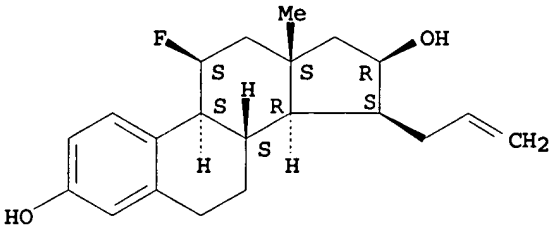
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-propyl-, (11β,15β,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



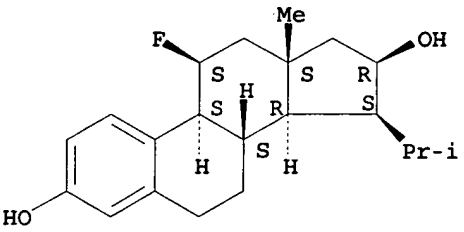
RN 287723-18-6 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(2-propenyl)-, (11β,15β,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



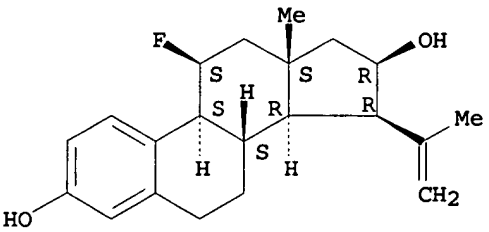
RN 287723-19-7 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(1-methylethyl)-, (11β,15β,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



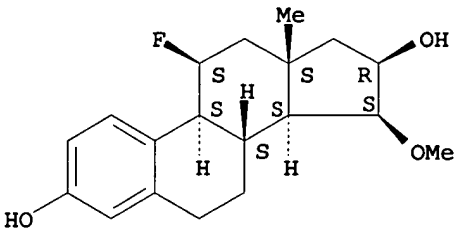
RN 287723-20-0 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(1-methylethenyl)-, (11β,15β,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



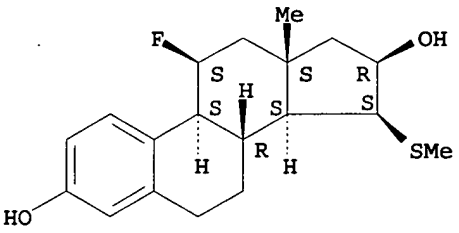
RN 287723-21-1 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-methoxy-, (11β,15β,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



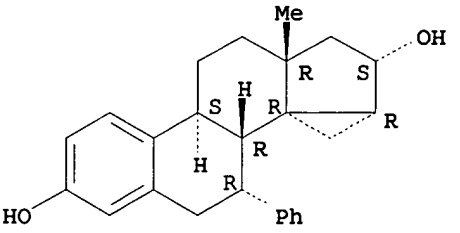
RN 287723-22-2 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(methylthio)-, (11β,15β,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



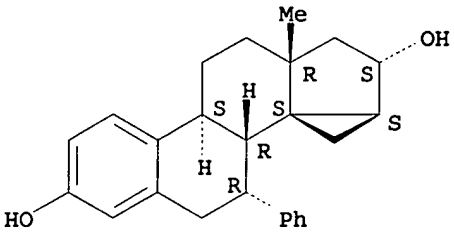
RN 287723-23-3 HCAPLUS
CN Cycloprop[14,15]estra-1,3,5(10)-triene-3,16-diol, 3',15-dihydro-7-phenyl-, (7α,14R,15β,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



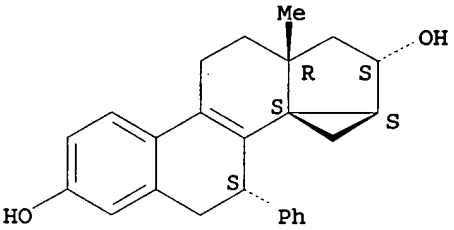
RN 287723-24-4 HCAPLUS
CN Cycloprop[14,15]estra-1,3,5(10)-triene-3,16-diol, 3',15-dihydro-7-phenyl-, (7α,14S,15α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



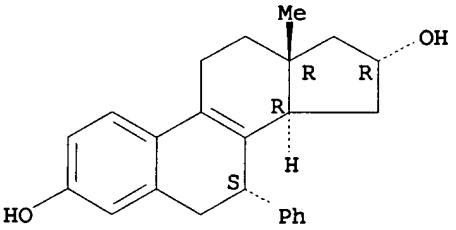
RN 287723-25-5 HCAPLUS
CN Cycloprop[14,15]estra-1,3,5(10),8-tetraene-3,16-diol, 3',15-dihydro-7-phenyl-, (7α,14S,15α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



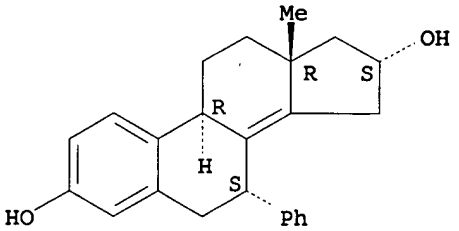
RN 287723-26-6 HCAPLUS
CN Estra-1,3,5(10),8-tetraene-3,16-diol, 7-phenyl-, (7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 287723-27-7 HCAPLUS
CN Estra-1,3,5(10),8(14)-tetraene-3,16-diol, 7-phenyl-, (7α,16α)- (9CI) (CA INDEX NAME)

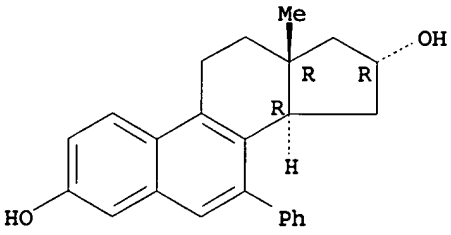
Absolute stereochemistry.



RN 287723-28-8 HCAPLUS
CN Estra-1,3,5,7,9-pentaene-3,16-diol, 7-phenyl-, (16α)- (9CI)

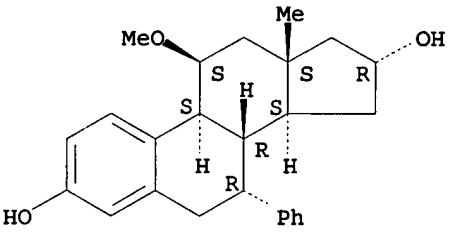
(CA INDEX NAME)

Absolute stereochemistry.



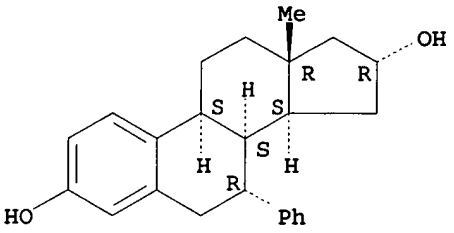
RN 287723-29-9 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-methoxy-7-phenyl-, (7α,11β,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



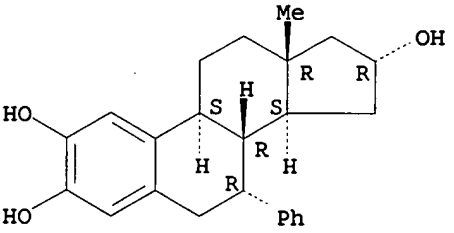
RN 287723-30-2 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 7-phenyl-, (7α,8α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



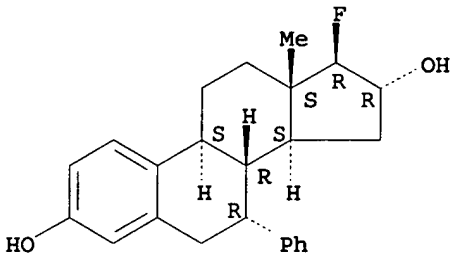
RN 287723-31-3 HCAPLUS
CN Estra-1,3,5(10)-triene-2,3,16-triol, 7-phenyl-, (7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



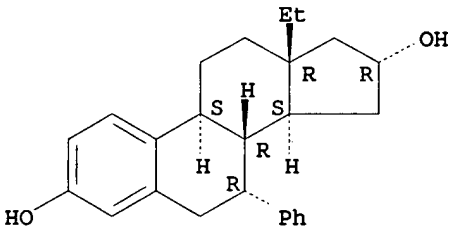
RN 287723-32-4 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 17-fluoro-7-phenyl-, (7α,16α,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



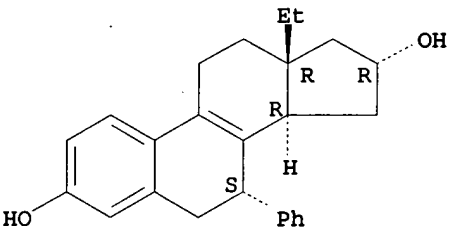
RN 287723-33-5 HCAPLUS
CN Gona-1,3,5(10)-triene-3,16-diol, 13-ethyl-7-phenyl-, (7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



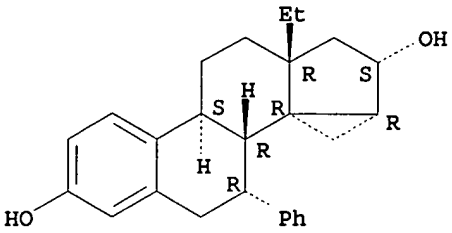
RN 287723-35-7 HCAPLUS
CN Gona-1,3,5(10),8-tetraene-3,16-diol, 13-ethyl-7-phenyl-, (7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



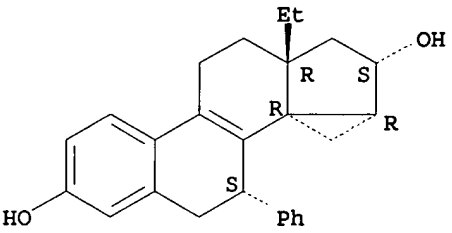
RN 287723-37-9 HCAPLUS
CN Cyclopropa[14,15]gona-1,3,5(10)-triene-3,16-diol, 13-ethyl-3',15-dihydro-7-phenyl-, (7α,14R,15β,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



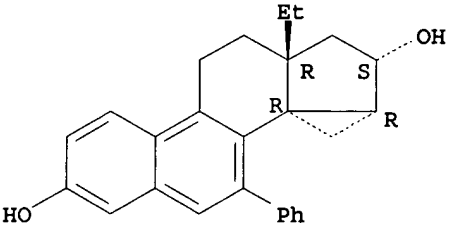
RN 287723-40-4 HCAPLUS
CN Cyclopropa[14,15]gona-1,3,5(10),8-tetraene-3,16-diol, 13-ethyl-3',15-dihydro-7-phenyl-, (7α,14R,15β,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



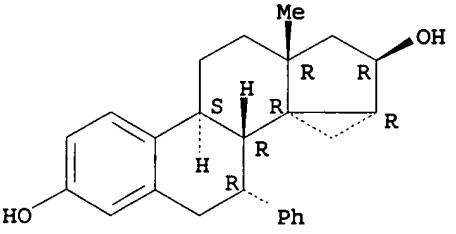
RN 287723-41-5 HCAPLUS
CN Cyclopropa[14,15]gona-1,3,5,7,9-pentaene-3,16-diol, 13-ethyl-3',15-dihydro-7-phenyl-, (14R,15β,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



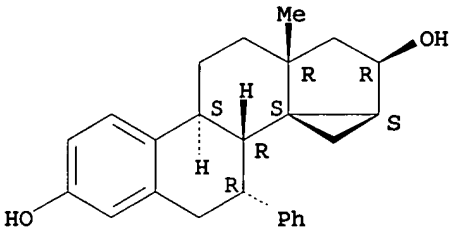
RN 287723-42-6 HCAPLUS
CN Cycloprop[14,15]estra-1,3,5(10)-triene-3,16-diol, 3',15-dihydro-7-phenyl-, (7α,14R,15β,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



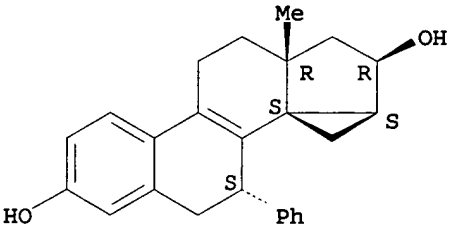
RN 287723-43-7 HCAPLUS
CN Cycloprop[14,15]estra-1,3,5(10)-triene-3,16-diol, 3',15-dihydro-7-phenyl-, (7α,14S,15α,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



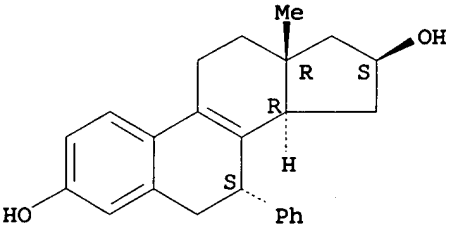
RN 287723-44-8 HCAPLUS
CN Cycloprop[14,15]estra-1,3,5(10),8-tetraene-3,16-diol, 3',15-dihydro-7-phenyl-, (7α,14S,15α,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



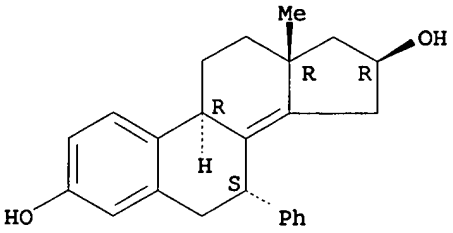
RN 287723-45-9 HCAPLUS
CN Estra-1,3,5(10),8-tetraene-3,16-diol, 7-phenyl-, (7α,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



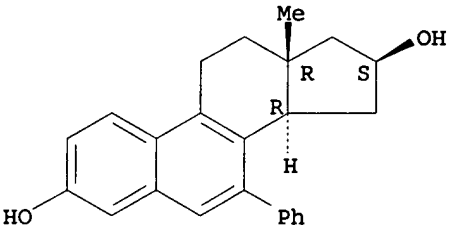
RN 287723-46-0 HCAPLUS
CN Estra-1,3,5(10),8(14)-tetraene-3,16-diol, 7-phenyl-, (7α,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



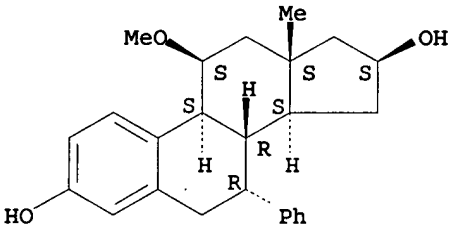
RN 287723-47-1 HCAPLUS
CN Estra-1,3,5,7,9-pentaene-3,16-diol, 7-phenyl-, (16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



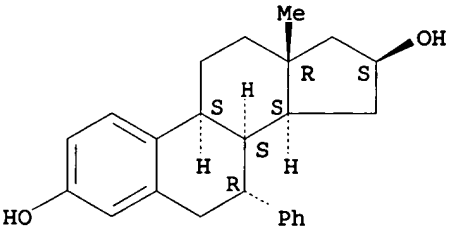
RN 287723-48-2 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-methoxy-7-phenyl-, (7α,11β,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



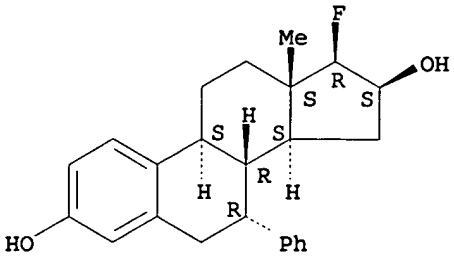
RN 287723-49-3 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 7-phenyl-, (7α,8α,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



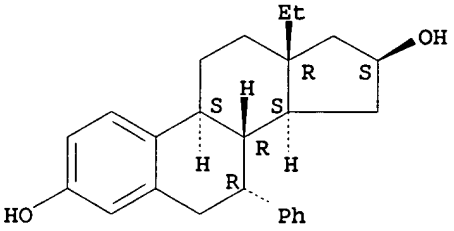
RN 287723-50-6 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 17-fluoro-7-phenyl-, (7α,16β,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



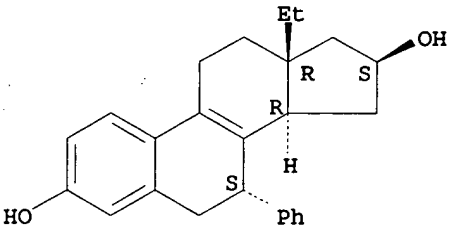
RN 287723-51-7 HCAPLUS
CN Gona-1,3,5(10)-triene-3,16-diol, 13-ethyl-7-phenyl-, (7α,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



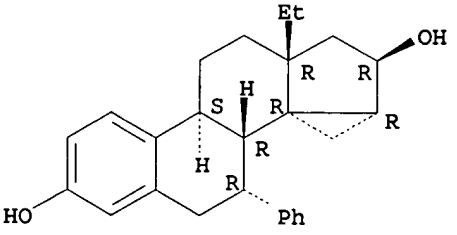
RN 287723-52-8 HCAPLUS
CN Gona-1,3,5(10),8-tetraene-3,16-diol, 13-ethyl-7-phenyl-, (7α,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



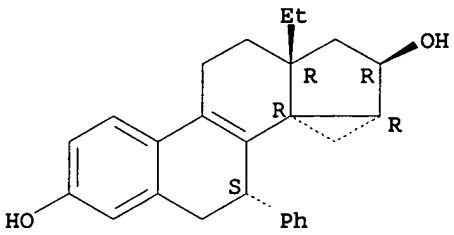
RN 287723-53-9 HCAPLUS
CN Cyclopropa[14,15]gona-1,3,5(10)-triene-3,16-diol, 13-ethyl-3',15-dihydro-7-phenyl-, (7α,14R,15β,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



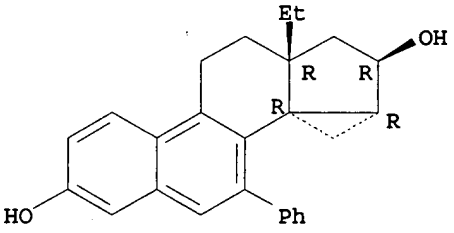
RN 287723-54-0 HCAPLUS
CN Cyclopropa[14,15]gona-1,3,5(10),8-tetraene-3,16-diol, 13-ethyl-3',15-dihydro-7-phenyl-, (7α,14R,15β,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



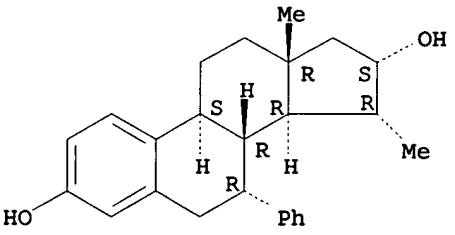
RN 287723-55-1 HCAPLUS
CN Cyclopropa[14,15]gona-1,3,5,7,9-pentaene-3,16-diol, 13-ethyl-3',15-dihydro-7-phenyl-, (14R,15β,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



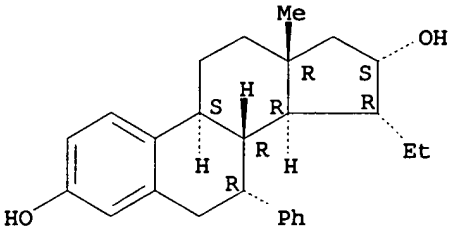
RN 287723-56-2 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 15-methyl-7-phenyl-, (7α,15α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



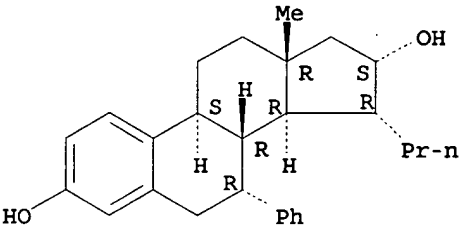
RN 287723-57-3 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 15-ethyl-7-phenyl-, (7α,15α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



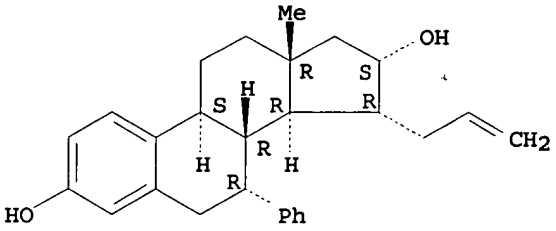
RN 287723-58-4 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 7-phenyl-15-propyl-, (7α,15α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



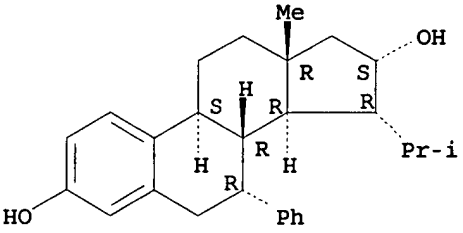
RN 287723-59-5 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 7-phenyl-15-(2-propenyl)-, (7α,15α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



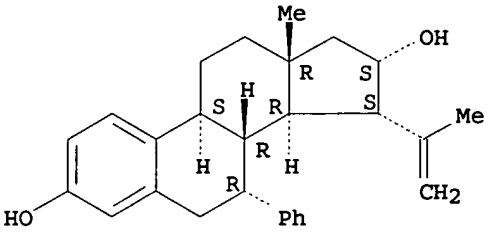
RN 287723-60-8 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 15-(1-methylethyl)-7-phenyl-, (7α,15α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



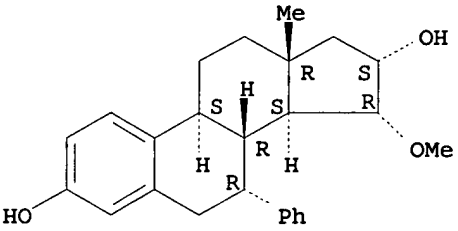
RN 287723-61-9 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 15-(1-methylethenyl)-7-phenyl-, (7α,15α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



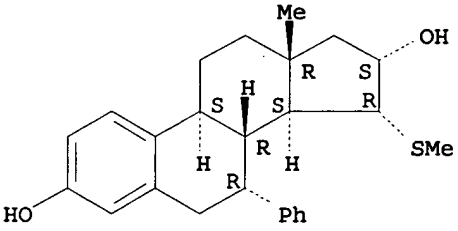
RN 287723-62-0 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 15-methoxy-7-phenyl-, (7α,15α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



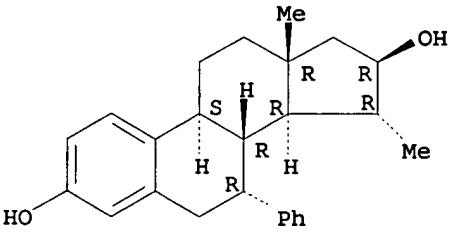
RN 287723-63-1 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 15-(methylthio)-7-phenyl-, (7α,15α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 287723-64-2 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 15-methyl-7-phenyl-, (7α,15α,16β)- (9CI) (CA INDEX NAME)

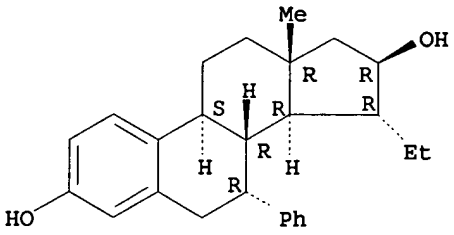
Absolute stereochemistry.



RN 287723-65-3 HCAPLUS

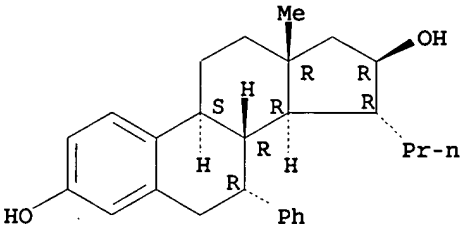
CN Estra-1,3,5(10)-triene-3,16-diol, 15-ethyl-7-phenyl-,
(7α,15α,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



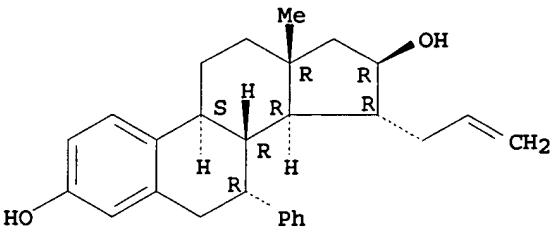
RN 287723-66-4 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 7-phenyl-15-propyl-,
(7α,15α,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



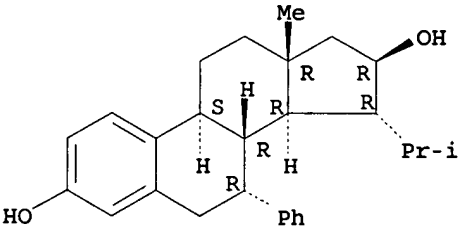
RN 287723-67-5 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 7-phenyl-15-(2-propenyl)-,
(7α,15α,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



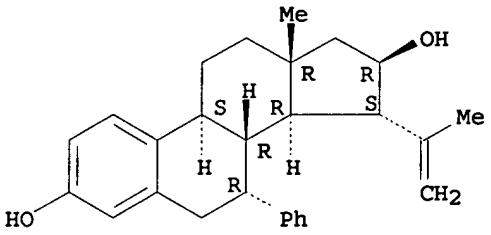
RN 287723-68-6 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 15-(1-methylethyl)-7-phenyl-,
(7α,15α,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



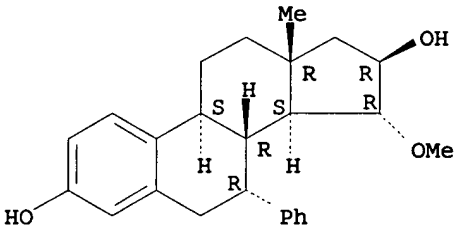
RN 287723-69-7 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 15-(1-methylethenyl)-7-phenyl-, (7α,15α,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



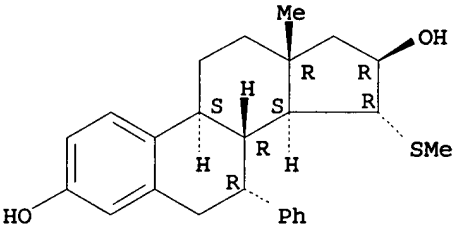
RN 287723-70-0 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 15-methoxy-7-phenyl-, (7α,15α,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



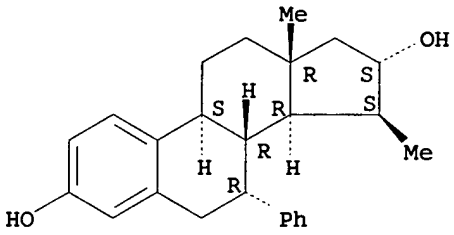
RN 287723-71-1 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 15-(methylthio)-7-phenyl-, (7α,15α,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



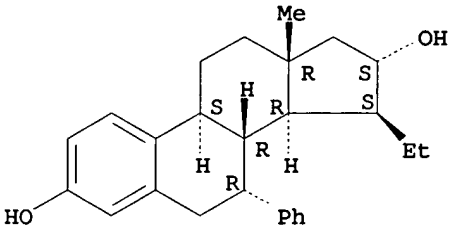
RN 287723-72-2 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 15-methyl-7-phenyl-, (7α,15β,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



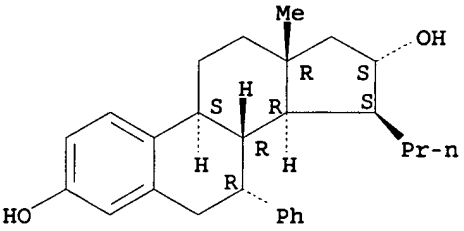
RN 287723-73-3 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 15-ethyl-7-phenyl-, (7α,15β,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



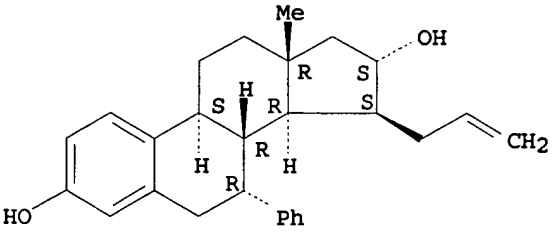
RN 287723-75-5 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 7-phenyl-15-propyl-, (7α,15β,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



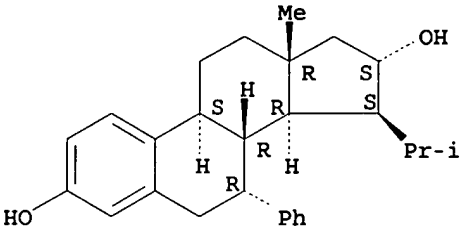
RN 287723-77-7 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 7-phenyl-15-(2-propenyl)-, (7α,15β,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



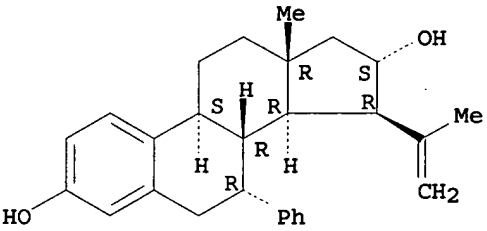
RN 287723-79-9 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 15-(1-methylethyl)-7-phenyl-, (7α,15β,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



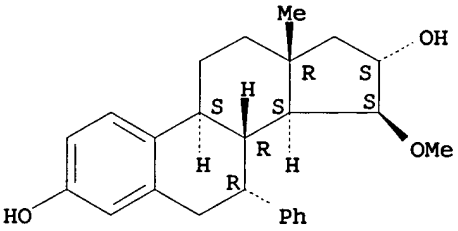
RN 287723-80-2 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 15-(1-methylethenyl)-7-phenyl-, (7α,15β,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



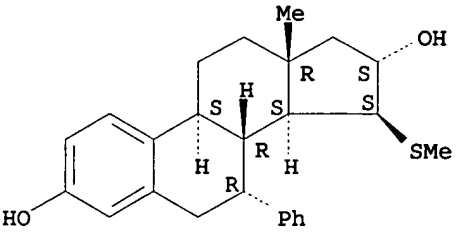
RN 287723-81-3 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 15-methoxy-7-phenyl-, (7α,15β,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 287723-82-4 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 15-(methylthio)-7-phenyl-, (7α,15β,16α)- (9CI) (CA INDEX NAME)

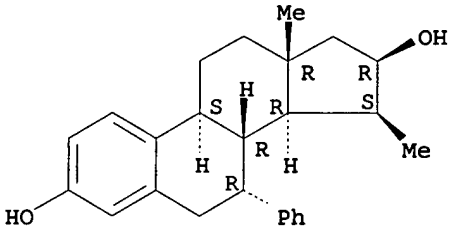
Absolute stereochemistry.



RN 287723-83-5 HCAPLUS

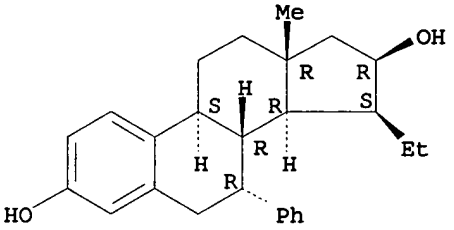
CN Estra-1,3,5(10)-triene-3,16-diol, 15-methyl-7-phenyl-, (7α,15β,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



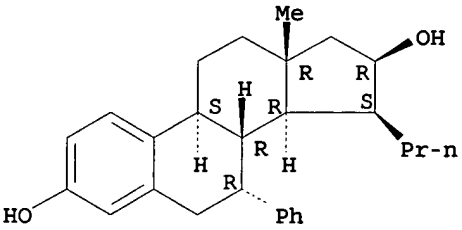
RN 287723-84-6 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 15-ethyl-7-phenyl-, (7α,15β,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



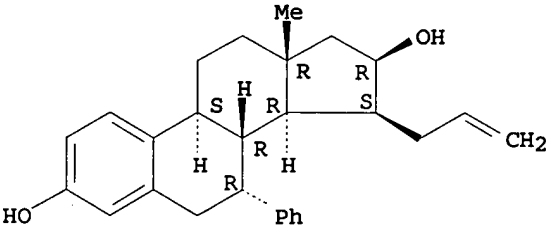
RN 287723-85-7 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 7-phenyl-15-propyl-, (7α,15β,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



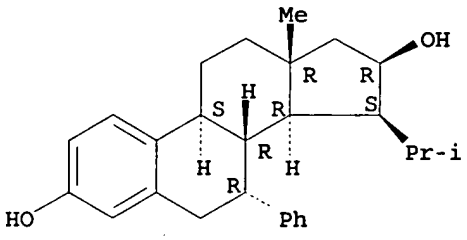
RN 287723-86-8 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 7-phenyl-15-(2-propenyl)-, (7α,15β,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



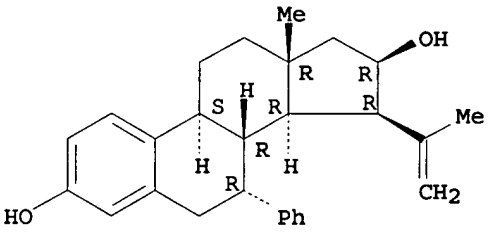
RN 287723-87-9 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 15-(1-methylethyl)-7-phenyl-, (7α,15β,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



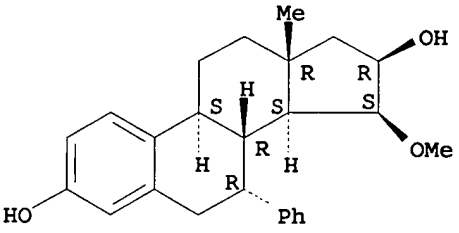
RN 287723-88-0 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 15-(1-methylethenyl)-7-phenyl-, (7α,15β,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



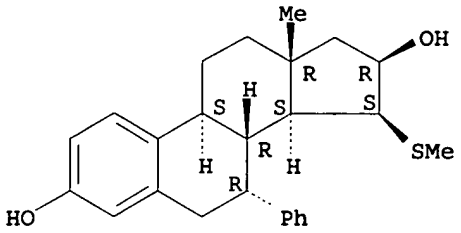
RN 287723-89-1 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 15-methoxy-7-phenyl-, (7α,15β,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



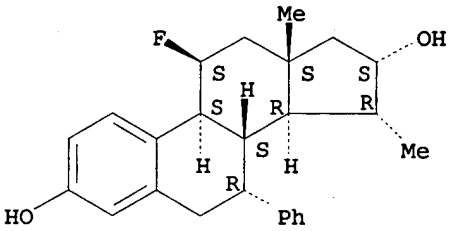
RN 287723-90-4 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 15-(methylthio)-7-phenyl-, (7α,15β,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



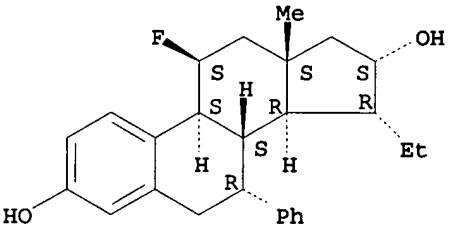
RN 287723-91-5 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-methyl-7-phenyl-, (7α,11β,15α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 287723-92-6 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 15-ethyl-11-fluoro-7-phenyl-, (7α,11β,15α,16α)- (9CI) (CA INDEX NAME)

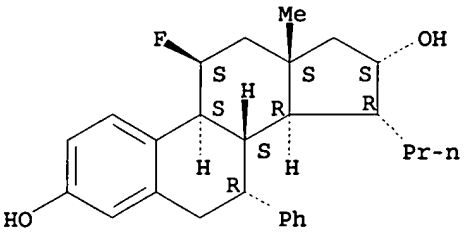
Absolute stereochemistry.



IT **287723-93-7P 287723-94-8P 287723-95-9P**
287723-96-0P 287723-97-1P 287723-98-2P
287723-99-3P 287724-00-9P 287724-01-0P
287724-02-1P 287724-03-2P 287724-04-3P
287724-05-4P 287724-06-5P 287724-07-6P
287724-08-7P 287724-09-8P 287724-10-1P
287724-11-2P 287724-12-3P 287724-13-4P
287724-14-5P 287724-15-6P 287724-16-7P
287724-17-8P 287724-18-9P 287724-19-0P
287724-20-3P 287724-21-4P 287724-22-5P
287724-23-6P 287724-24-7P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis of 16-Hydroxyestratrienes as selectively effective **estrogens**)

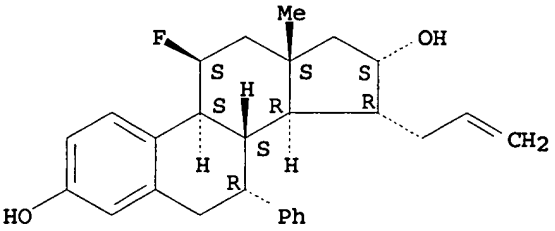
RN 287723-93-7 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-phenyl-15-propyl-, (7α,11β,15α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



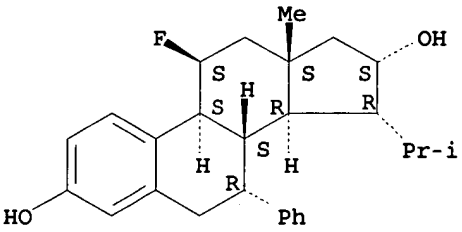
RN 287723-94-8 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-phenyl-15-(2-propenyl)-, (7α,11β,15α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



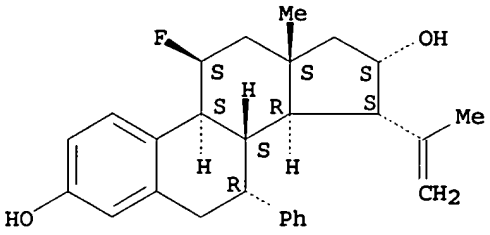
RN 287723-95-9 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(1-methylethyl)-7-phenyl-, (7α,11β,15α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



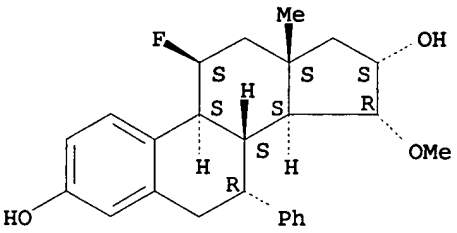
RN 287723-96-0 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(1-methylethenyl)-7-phenyl-, (7α,11β,15α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



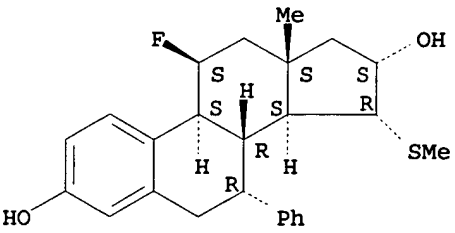
RN 287723-97-1 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-methoxy-7-phenyl-, (7α,11β,15α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



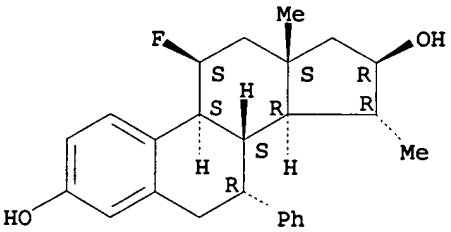
RN 287723-98-2 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(methylthio)-7-phenyl-, (7α,11β,15α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 287723-99-3 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-methyl-7-phenyl-, (7α,11β,15α,16β)- (9CI) (CA INDEX NAME)

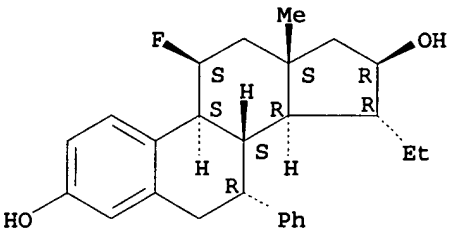
Absolute stereochemistry.



RN 287724-00-9 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 15-ethyl-11-fluoro-7-phenyl-,

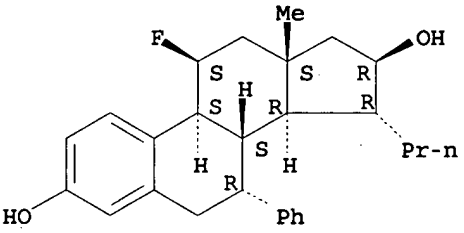
(7α,11β,15α,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



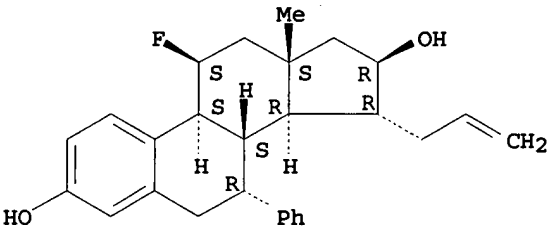
RN 287724-01-0 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-phenyl-15-propyl-, (7α,11β,15α,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



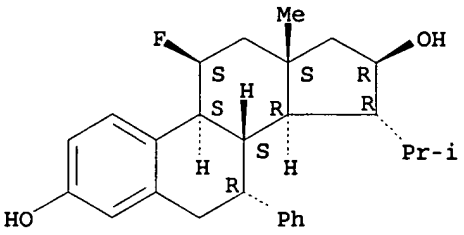
RN 287724-02-1 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-phenyl-15-(2-propenyl)-, (7α,11β,15α,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



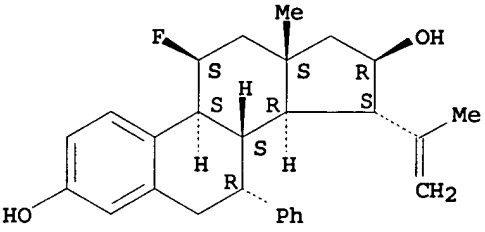
RN 287724-03-2 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(1-methylethyl)-7-phenyl-, (7α,11β,15α,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



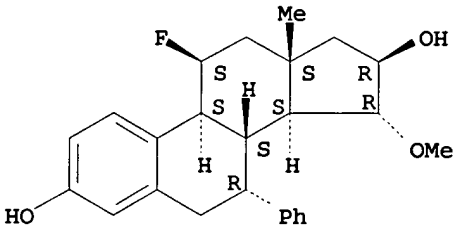
RN 287724-04-3 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(1-methylethenyl)-7-phenyl-, (7α,11β,15α,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



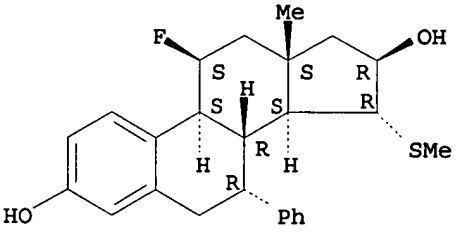
RN 287724-05-4 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-methoxy-7-phenyl-, (7α,11β,15α,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 287724-06-5 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(methylthio)-7-phenyl-, (7α,11β,15α,16β)- (9CI) (CA INDEX NAME)

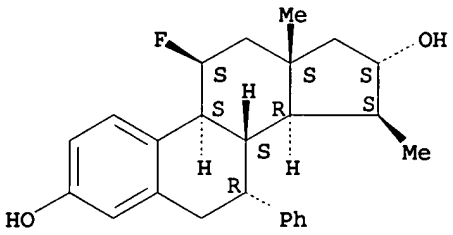
Absolute stereochemistry.



RN 287724-07-6 HCAPLUS

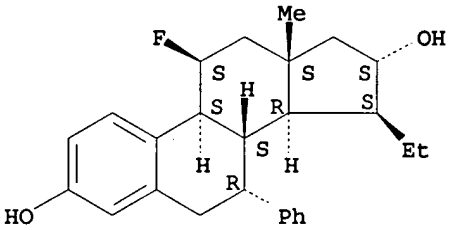
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-methyl-7-phenyl-, (7α,11β,15β,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



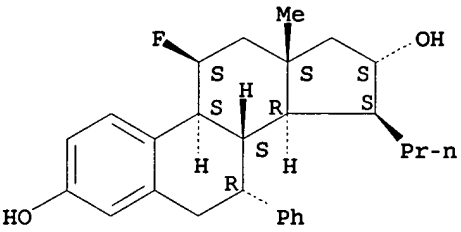
RN 287724-08-7 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 15-ethyl-11-fluoro-7-phenyl-, (7α,11β,15β,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



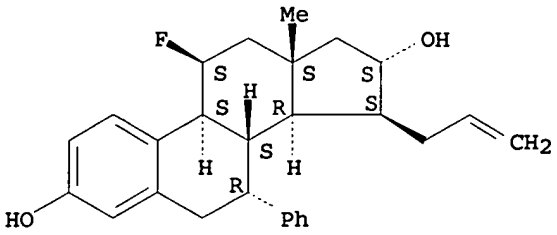
RN 287724-09-8 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-phenyl-15-propyl-, (7α,11β,15β,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



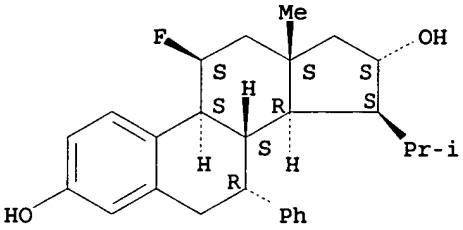
RN 287724-10-1 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-phenyl-15-(2-propenyl)-, (7α,11β,15β,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



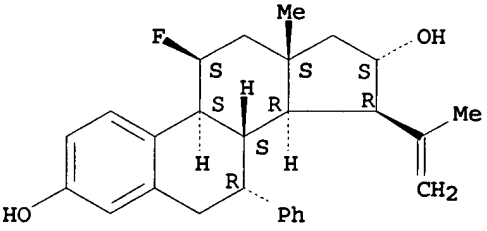
RN 287724-11-2 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(1-methylethyl)-7-phenyl-, (7α,11β,15β,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



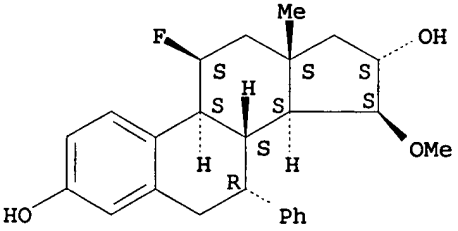
RN 287724-12-3 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(1-methylethenyl)-7-phenyl-, (7α,11β,15β,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 287724-13-4 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-methoxy-7-phenyl-, (7α,11β,15β,16α)- (9CI) (CA INDEX NAME)

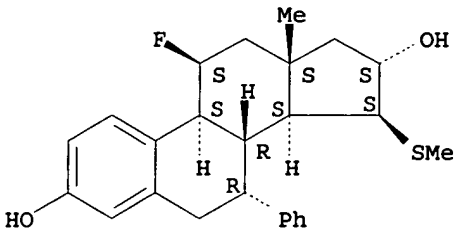
Absolute stereochemistry.



RN 287724-14-5 HCAPLUS

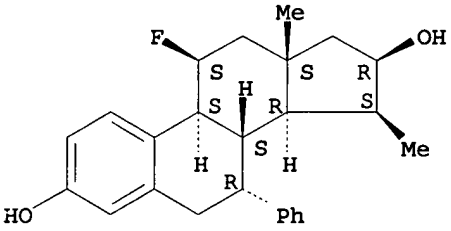
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(methylthio)-7-phenyl-, (7α,11β,15β,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



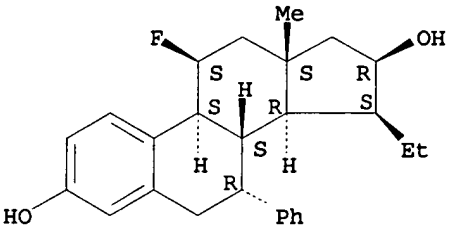
RN 287724-15-6 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-methyl-7-phenyl-, (7α,11β,15β,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



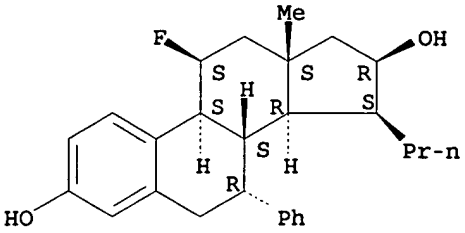
RN 287724-16-7 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 15-ethyl-11-fluoro-7-phenyl-, (7α,11β,15β,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



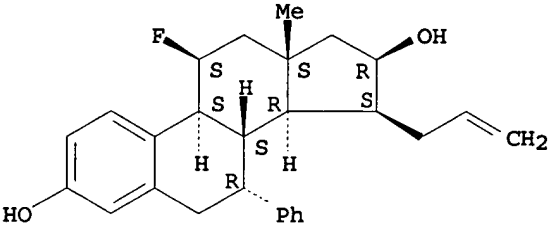
RN 287724-17-8 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-phenyl-15-propyl-, (7α,11β,15β,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



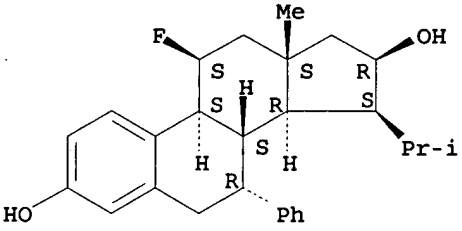
RN 287724-18-9 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-phenyl-15-(2-propenyl)-, (7α,11β,15β,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



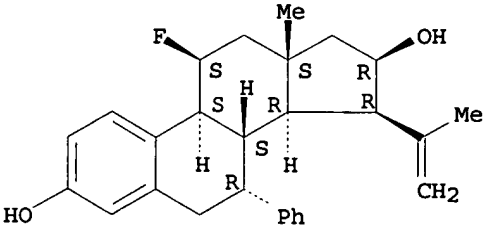
RN 287724-19-0 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(1-methylethyl)-7-phenyl-, (7α,11β,15β,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



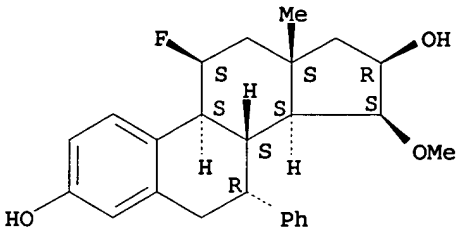
RN 287724-20-3 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(1-methylethenyl)-7-phenyl-, (7α,11β,15β,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



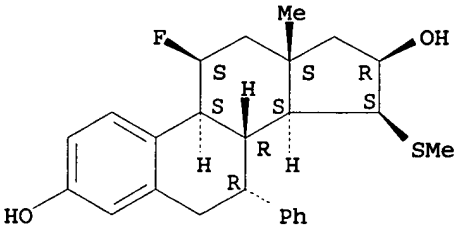
RN 287724-21-4 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-methoxy-7-phenyl-, (7α,11β,15β,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



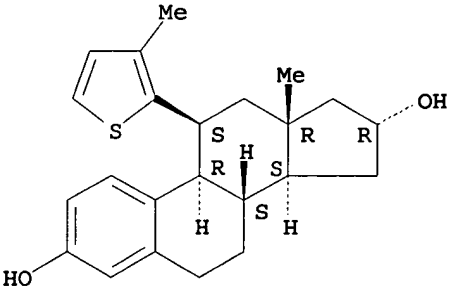
RN 287724-22-5 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(methylthio)-7-phenyl-, (7α,11β,15β,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



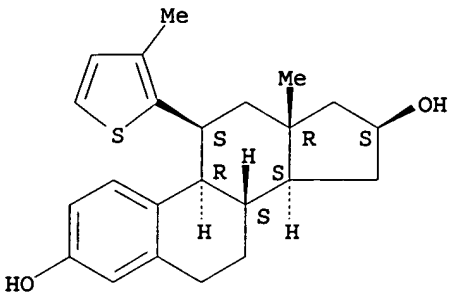
RN 287724-23-6 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-(3-methyl-2-thienyl)-, (11β,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



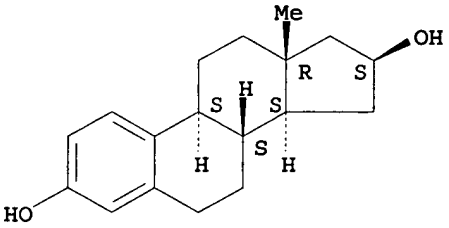
RN 287724-24-7 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 11-(3-methyl-2-thienyl)-, (11β,16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **1225-58-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis of 16-Hydroxyestratrienes as selectively effective **estrogens**)
RN 1225-58-7 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, (16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC ICM C07J009-00
ICS C07J001-00; A61K031-565; A61K031-575
CC 32-3 (**Steroids**)
Section cross-reference(s): **1**, **63**
ST estratriene hydroxy analog prepn **estrogen** therapy
IT Prostate gland
(benign hyperplasia; synthesis of 16-Hydroxyestratrienes as selectively effective **estrogens**)
IT Uterus, neoplasm
(cervix, carcinoma, intraepithelial; synthesis of 16-Hydroxyestratrienes as selectively effective **estrogens**)
IT **Estrogens**
(deficiency; synthesis of 16-Hydroxyestratrienes as selectively effective **estrogens**)
IT Nervous system
(degeneration; synthesis of 16-Hydroxyestratrienes as selectively effective **estrogens**)
IT Immunity
(disorder; synthesis of 16-Hydroxyestratrienes as selectively effective **estrogens**)
IT Fertility
(female, disorder; synthesis of 16-Hydroxyestratrienes as selectively effective **estrogens**)
IT Artery, disease
(intima, hyperplasia; synthesis of 16-Hydroxyestratrienes as selectively effective **estrogens**)
IT Fertility
(male, disorder; synthesis of 16-Hydroxyestratrienes as selectively effective **estrogens**)
IT Menopause

(perimenopause; synthesis of 16-Hydroxyestratrienes as selectively effective **estrogens**)
IT Menopause
(postmenopause; synthesis of 16-Hydroxyestratrienes as selectively effective **estrogens**)
IT Alzheimer's disease
Arteriosclerosis
Blood vessel, disease
Heart, disease
Hormone replacement therapy
Ovary, disease
(synthesis of 16-Hydroxyestratrienes as selectively effective **estrogens**)
IT Osteoporosis
(therapeutic agents; synthesis of 16-Hydroxyestratrienes as selectively effective **estrogens**)
IT **109932-04-9P 110012-46-9P 287721-55-5P**
287721-56-6P 287721-57-7P 287721-58-8P
287721-59-9P 287721-60-2P 287721-61-3P
287721-62-4P 287721-63-5P 287721-64-6P
287721-65-7P 287721-66-8P 287721-67-9P
287721-68-0P 287721-69-1P 287721-70-4P
287721-71-5P 287721-72-6P 287721-73-7P
287721-74-8P 287721-75-9P 287721-76-0P
287721-77-1P 287721-78-2P 287721-79-3P
287721-80-6P 287721-81-7P 287721-82-8P
287721-83-9P 287721-84-0P 287721-85-1P
287721-86-2P 287721-87-3P 287721-88-4P
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287721-92-0P 287721-93-1P 287721-94-2P
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287723-87-9P 287723-88-0P 287723-89-1P
287723-90-4P 287723-91-5P 287723-92-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis of 16-Hydroxyestratrienes as selectively effective **estrogens**)

IT **287723-93-7P 287723-94-8P 287723-95-9P**
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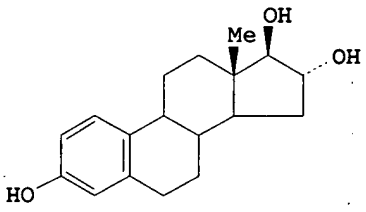
287723-99-3P 287724-00-9P 287724-01-0P
287724-02-1P 287724-03-2P 287724-04-3P
287724-05-4P 287724-06-5P 287724-07-6P
287724-08-7P 287724-09-8P 287724-10-1P
287724-11-2P 287724-12-3P 287724-13-4P
287724-14-5P 287724-15-6P 287724-16-7P
287724-17-8P 287724-18-9P 287724-19-0P
287724-20-3P 287724-21-4P 287724-22-5P
287724-23-6P 287724-24-7P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis of 16-Hydroxyestratrienes as selectively effective **estrogens**)

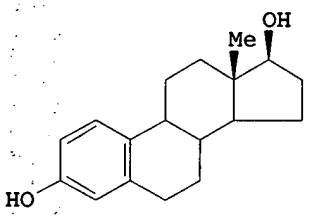
IT **1225-58-7** 10449-00-0 13639-96-8 13865-88-8
59126-71-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis of 16-Hydroxyestratrienes as selectively effective **estrogens**)

IT 287724-25-8P 287724-26-9P 287724-27-0P 287724-28-1P
287724-29-2P 287724-30-5P 287724-31-6P 287724-32-7P
287724-33-8P 287724-34-9P 287724-35-0P 287724-36-1P
287724-37-2P 287724-38-3P 287724-39-4P 287724-40-7P
287724-41-8P 287724-42-9P 287726-67-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of 16-Hydroxyestratrienes as selectively effective **estrogens**)

L52 ANSWER 2 OF 24 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1990:801 HCAPLUS
DOCUMENT NUMBER: 112:801
TITLE: Relative mitogenic activities of various estrogens and antiestrogens
AUTHOR(S): Stack, Gary; Korach, Kenneth; Gorski, Jack
CORPORATE SOURCE: Coll. Agric. Life Sci., Univ. Wisconsin, Madison, WI, 53706, USA
SOURCE: Steroids (1989), 54(2), 227-43
CODEN: STEDAM; ISSN: 0039-128X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

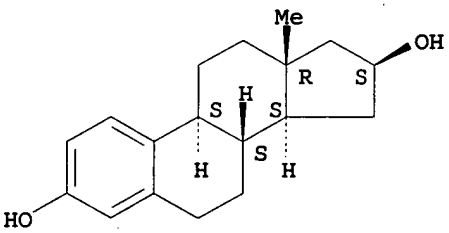


II

AB The abilities of a variety of estrogens and antiestrogens to stimulate DNA synthesis in the prepuberal rat uterus were compared. One microgram of each compound was administered in vivo via a single i.p. injection. DNA synthesis was assayed in vitro in isolated nuclei 24 h later. The relative mitogenicities of the steroidal estrogens were : 16α-estradiol < 17α-estradiol = estriol (I) = 16-epiestriol < 16β-estradiol = 17β-estradiol (II). The potencies of several nonsteroidal estrogens were also tested. Indenestrol A was as potent as II, whereas indanestrol and dimethylstilbestrol had weaker activities. The antiestrogens, nafoxidine and 4-hydroxytamoxifen, were both potent stimulators of DNA synthesis. The abilities of an estrogen to stimulate increases in uterine wet weight, DNA polymerase α activities, and DNA synthesis in uterine nuclei 24 h after injection were closely correlated. Because the magnitude of the stimulation of DNA synthesis was greatest, its measurement is the most sensitive of these assays, of uterotropic activity.

IT **1225-58-7**, 16β-Estradiol
RL: PROC (Process)
(mitogenic action of, on uterus, mol. structure in relation to)
RN 1225-58-7 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, (16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 2-2 (Mammalian Hormones)
IT 50-27-1 50-28-2, Estradiol, biological studies 57-91-0,

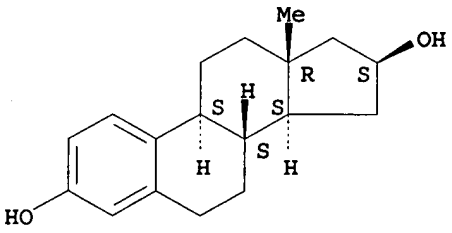
17α-Estradiol 547-81-9 552-80-7, Dimethylstilbestrol
1090-04-6, 16α-Estradiol **1225-58-7**,
16β-Estradiol 1845-11-0, Nafoxidine 24643-97-8
68047-06-3 71855-45-3, Indanestrol
RL: PROC (Process)
(mitogenic action of, on uterus, mol. structure in relation to)

L52 ANSWER 3 OF 24 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1988:622771 HCAPLUS
DOCUMENT NUMBER: 109:222771
TITLE: Effect of endogenous and synthetic sex steroids on the clearance of antibody-coated cells
AUTHOR(S): Schreiber, A. D.; Nettl, F. M.; Sanders, M. C.; King, M.; Szabolcs, P.; Friedman, D.; Gomez, F.
CORPORATE SOURCE: Cancer Cent., Univ. Pennsylvania, Philadelphia, PA, 19104, USA
SOURCE: Journal of Immunology (1988), 141(9), 2959-66
CODEN: JOIMA3; ISSN: 0022-1767
DOCUMENT TYPE: Journal
LANGUAGE: English

AB An exptl. model developed in the guinea pig, was used to study the effects of female sex hormones on macrophage clearance of IgG- and IgM-coated erythrocytes in the spleen and liver. Progesterone, its naturally occurring analog 17-hydroxyprogesterone, and its synthetic analog 16-methylprogesterone inhibited the clearance of IgG-coated erythrocytes by splenic macrophages. Furthermore, when splenic macrophages were isolated from progesterone-treated animals they expressed decreased FcγR activity. Estradiol, estriol, and the estrogen analog 1,3,5(10)-estratriene-3,16β-diol enhanced splenic macrophage clearance of IgG-coated erythrocytes. This action of the estrogens could be partially inhibited by the antiestrogen tamoxifen. However, estradiol did not affect the C3-dependent clearance of IgM-coated erythrocytes by hepatic macrophages. Concurrent administration of estradiol and progesterone demonstrated that the action of estradiol was predominant. Thus, female sex hormones alter splenic macrophage FcγR function at concns. observed during the human menstrual cycle and pregnancy. This result may also explain alteration of disease activity in some human immunol. disorders during changes in the hormonal states.

IT **1225-58-7**
RL: BIOL (Biological study)
(IgG-coated erythrocyte clearance by spleen macrophage stimulation by)
RN 1225-58-7 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, (16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

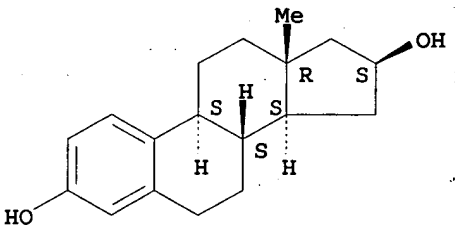


CC 2-4 (Mammalian Hormones)
Section cross-reference(s): 15
IT 50-27-1, Estriol 50-28-2, Estradiol, biological studies

1225-58-7
RL: BIOL (Biological study)
(IgG-coated erythrocyte clearance by spleen macrophage stimulation by)

L52 ANSWER 4 OF 24 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1987:96443 HCAPLUS
DOCUMENT NUMBER: 106:96443
TITLE: Influence of adrenergic receptors on ovarian progesterone secretion in the pseudopregnant cat and estradiol secretion in the estrous cat
AUTHOR(S): Wheeler, A. G.; Walker, M.; Lean, J.
CORPORATE SOURCE: Dep. Physiol. Pharmacol., Univ. Queensland, St. Lucia, 4067, Australia
SOURCE: Journal of Reproduction and Fertility (1987), 79(1), 195-205
CODEN: JRPFA4; ISSN: 0022-4251
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The infusion of isoprenaline [7683-59-2] or propranolol into the abdominal aorta of the pseudopregnant cat caused an increase or decrease, resp., in the ovarian progesterone [57-83-0] secretion rate. Apparently, the sympathetic innervation of the ovary has a physiol. influence on normal progesterone secretion, and this mechanism may explain stress-related increases in progesterone concns. The infusion of isoprenaline or propranolol after the stimulation of follicular growth had no consistent or convincing effect on estradiol [**1225-58-7**] secretion.
IT **1225-58-7**
RL: PROC (Process)
(secretion of, by ovary, adrenergic receptors in relation to)
RN 1225-58-7 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, (16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 2-4 (Mammalian Hormones)
IT **1225-58-7**
RL: PROC (Process)
(secretion of, by ovary, adrenergic receptors in relation to)

L52 ANSWER 5 OF 24 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1987:16187 HCAPLUS
DOCUMENT NUMBER: 106:16187
TITLE: Methylcholanthrene: a possible pseudosubstrate for adrenocortical 17α-hydroxylase and aryl hydrocarbon hydroxylase
AUTHOR(S): Hornsby, Peter J.; Aldern, Kathy A.; Harris, Sandra E.
CORPORATE SOURCE: Sch. Med., Univ. California, La Jolla, CA, 92093, USA
SOURCE: Biochemical Pharmacology (1986), 35(19), 3209-19

CODEN: BCPCA6; ISSN: 0006-2952
DOCUMENT TYPE: Journal
LANGUAGE: English

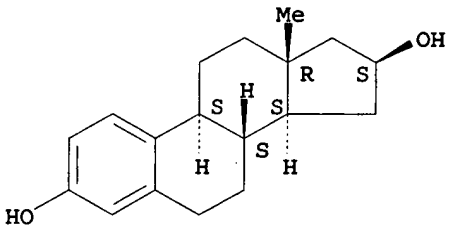
AB In cultured bovine adrenocortical cells, the loss of steroid 17α-hydroxylase (I) activity was observed after incubation with 3-methylcholanthrene (3-MC). The suppression of I by 3-MC was rapid (50% loss of activity in 10 h at 1 μm 3-MC), did not exhibit a lag period, and was not affected by cycloheximide. Direct effects of 3-MC on I were observed only at high concns., but the concentration for 50% loss of activity was 0.3 μM when 3-MC was added for 24 h prior to assay of I. High concns. (to 40 μM) of substrate (progesterone), did not affect the loss of activity due to 3-MC. Loss of I activity was specific; steroid 11β-hydroxylase was unaffected and cell growth was unaltered. However, 22-amino-23,24-bisnorchol-5-en-3β-ol, an inhibitor of I, partially prevented the loss of I at 1-30 nM. 3-MC was thought to induce cytochrome P 450s via a receptor with high affinity for 2,3,7,8-tetrachlorodibenzo-p-dioxin (TCDD). TCDD was without effect on I over the range 10 nM-10 μM. Benz[a]anthracene, 7,12-dimethylbenz[a]anthracene, benzo[a]pyrene, chrysene, and methylphenanthrenes suppressed I at high concns. (10-50 μM for 50% loss of activity). Some steroids that lack a substituent at position 17 also caused loss of I. Like I, bovine adrenocortical cell aryl hydrocarbon hydroxylase (II) was found to be suppressed by exposure to 3-MC. Compds. that caused loss of I caused loss of II, with a similar order of potency and at similar concns. Suppression of II by 3-MC did not require protein synthesis and was prevented by an inhibitor of enzymic activity, α-naphthoflavone. This implied a degree of similarity of the cytochrome P 450s for I and II, but the activities were shown to be likely due to different enzymes. The suppression of I and II by 3-MC appeared not to occur by a receptor-mediated mechanism but to be similar to the suppression of steroid 11β-hydroxylase and steroid 21-hydroxylase by steroid pseudosubstrates previously observed

IT **1225-58-7**, Estra-1,3,5(10)-triene-3,16β-diol
RL: BIOL (Biological study)
(aryl hydrocarbon hydroxylase and steroid 17α-hydroxylase response to, in adrenocortical cells)

RN 1225-58-7 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



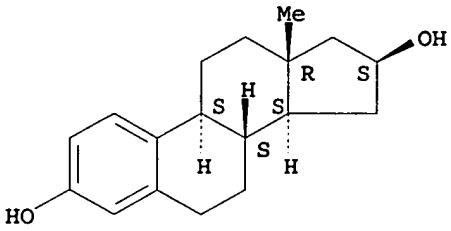
CC 13-2 (Mammalian Biochemistry)
Section cross-reference(s): 7

IT 50-32-8, Benz[a]pyrene, biological studies 56-49-5, 3-Methylcholanthrene 56-55-3, Benz[a]anthracene 57-97-6, 7,12-Dimethylbenz[a]anthracene 63-05-8, Androstenedione 218-01-9, Chrysene 832-69-9, 1-Methylphenanthrene 1153-51-1, 5α-Androst-16-en-3α-ol **1225-58-7**, Estra-1,3,5(10)-triene-3,16β-diol 2531-84-2, 2-Methylphenanthrene 7148-51-8, 5α-Androst-16-en-3β-ol 17012-89-4, 4-Methylcholanthrene 18339-16-7,

5α-Androst-16-en-3-one
RL: BIOL (Biological study)
(aryl hydrocarbon hydroxylase and steroid 17α-hydroxylase response to, in adrenocortical cells)

L52 ANSWER 6 OF 24 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1985:574487 HCAPLUS
DOCUMENT NUMBER: 103:174487
TITLE: Isolation of novel microbial 3α-, 3β-, and 17β-hydroxysteroid dehydrogenases. Purification, characterization, and analytical applications of a 17β-hydroxysteroid dehydrogenase from an Alcaligenes sp
AUTHOR(S): Payne, Donna W.; Talalay, Paul
CORPORATE SOURCE: Sch. Med., Johns Hopkins Univ., Baltimore, MD, 21205, USA
SOURCE: Journal of Biological Chemistry (1985), 260(25), 13648-55
CODEN: JBCHA3; ISSN: 0021-9258
DOCUMENT TYPE: Journal
LANGUAGE: English
AB By selecting for growth on testosterone or 17β-estradiol as the only source of organic C, a number of soil microorganisms which contain highly active and novel, inducible, NAD-linked 3α-, 3β-, and 17β-hydroxy steroid dehydrogenases were isolated. Such enzymes are suitable for the microanal. of steroids and of steroid-transforming enzymes, as well as for performing stereoselective oxidns. and reduction of steroids. Of particular interest among these organisms is a new species of Alcaligenes containing 17β-hydroxy steroid dehydrogenase (I) easily separable from 3β-hydroxy steroid dehydrogenase activity. Unlike any of the other isolated organisms, this Alcaligenes species contained no 3α-hydroxy steroid dehydrogenase activity. A large-scale purification (763-fold) to homogeneity of the major induced I was achieved by ion-exchange, hydrophobic, and affinity chromatogs. The enzyme has high specific activity for the oxidation of testosterone (Vmax = 303 μmol/min/mg protein; Km = 3.6 μM) and reacts almost equally well with 17β-estradiol (Vmax = 356 μmol/min/mg; Km = 6.4 μM). It consists of apparently identical subunits mol. weight = 32,000) and exists in polymeric form under nondenaturing conditions (mol. weight = 68,000 by gel filtration. and 86,000 by polyacrylamide gel electrophoresis). The isoelec. point is pH 5.1. The enzyme is almost completely specific for 17β-hydroxy steroids which may be Δ5-olefins or ring A phenols or have cis or trans A/B ring fusions. Substituents at other positions are tolerated, although the presence of a 16α- or 16β-OH group blocks the oxidation of the 17β-OH function. 3β-Hydroxy steroids (A/B ring fusion trans, but not cis, or Δ5-olefins) are very poor substrates. The application of this highly active, specific, and stable I to the microestn. of steroids by enzymic cycling of nicotinamide nucleotides and for the stereospecific oxidation of steroids is demonstrated.
IT **1225-58-7**
RL: BIOL (Biological study)
(17β-hydroxy steroid dehydrogenase of Alcaligenes specificity for, structure in relation to)
RN 1225-58-7 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, (16β)- (9CI) (CA INDEX NAME)

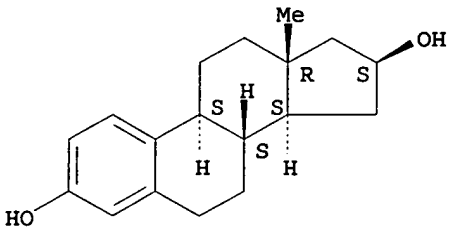
Absolute stereochemistry.



CC 7-2 (Enzymes)
Section cross-reference(s): 2, 9
IT 57-91-0 62-99-7 521-17-5 521-18-6 547-81-9 571-20-0
571-22-2 1156-92-9 **1225-58-7** 1816-85-9 1851-23-6
1852-53-5 2226-70-2 3066-12-4
RL: BIOL (Biological study)
(17β-hydroxy steroid dehydrogenase of Alcaligenes
specificity for, structure in relation to)

L52 ANSWER 7 OF 24 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1984:47664 HCAPLUS
DOCUMENT NUMBER: 100:47664
TITLE: Inhibitor specificity of the placental microsomal oxidase system responsible for the aromatization of epitestosterone (17α-hydroxy-4-androsten-3-one)
AUTHOR(S): Sheean, Leon A.; Meigs, Robert A.
CORPORATE SOURCE: Sch. Med., Case Western Reserve Univ., Cleveland, OH, 44106, USA
SOURCE: Steroids (1983), 41(2), 225-41
CODEN: STEDAM; ISSN: 0039-128X
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Human placental microsomes converted epitestosterone to 17α-estradiol at rates of 23-48 pmol/min/mg protein with a Km of 113 μM. The activity was inhibited 70-90% by concns. of CO, metyrapone, octylamine, 7,8-benzoflavone, and 7-ethoxycoumarin which had no effect on the aromatization of 4-androstene-3,17-dione. Conversely, CN- and N3- were more effective inhibitors of the conversion of the latter androgen. A variety of neutral steroids inhibited the aromatization of epitestosterone with 19-norsteroids being particularly effective, but competitive effects could not be demonstrated. Both 17β-hydroxy-4-estren-3-one and 16α-hydroxy-4-androstene-3,17-dione caused a mixed inhibition. A number of phenolic steroids were also inhibitory with 16-oxo compds. being particularly effective. Inhibition by estrone was non-competitive (Ki = 16 μM). The aromatization of epitestosterone resembles placental microsomal oxidase activities against estrone and benzo[a]pyrene in its inhibitor specificity and epitestosterone may be the native substrate for an oxidase also active in the metabolism of aromatic xenobiotic chems.
IT **1225-58-7**
RL: BIOL (Biological study)
(epitestosterone oxidase of human placenta microsomes inhibition by)
RN 1225-58-7 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, (16β)- (9CI) (CA INDEX NAME)

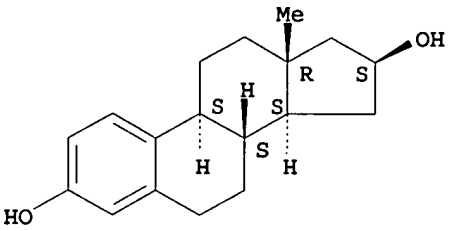
Absolute stereochemistry.



CC 7-3 (Enzymes)
IT 50-27-1 50-28-2, biological studies 53-16-7, biological studies 53-45-2 53-63-4 56-53-1 57-91-0 58-18-4 58-22-0 63-01-4 63-02-5 63-05-8 362-06-1 434-03-7 434-22-0 521-18-6 547-81-9 566-75-6 566-76-7 571-52-8 734-32-7 793-89-5 846-46-8 1089-78-7 1090-04-6 **1225-58-7** 1228-72-4 1228-73-5 1624-62-0 1743-60-8 3601-97-6 3646-30-8 3962-66-1 4011-48-7 6038-23-9 6132-10-1 6199-65-1
RL: BIOL (Biological study)
(epitestosterone oxidase of human placenta microsomes inhibition by)

L52 ANSWER 8 OF 24 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1981:561659 HCAPLUS
DOCUMENT NUMBER: 95:161659
TITLE: Characteristics of membrane transport of methotrexate by cultured human breast cancer cells
AUTHOR(S): Schilsky, Richard L.; Bailey, Brenda D.; Chabner, Bruce A.
CORPORATE SOURCE: Div. Cancer Treat., Natl. Cancer Inst., Bethesda, MD, 20205, USA
SOURCE: Biochemical Pharmacology (1981), 30(12), 1537-42
CODEN: BCPCA6; ISSN: 0006-2952
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Methotrexate (I) [59-05-2] transport by MCF-7 cells and cultured estrogen- and insulin [9004-10-8]-sensitive human breast cancer cells exhibited a high-affinity carrier system that displayed Michaelis-Menten kinetics (Km 8.22μM, Vmax 12.22 nmol/min/g cell protein), was competitively inhibited by leucovorin and aminopterin but not folic acid, and was temperature-sensitive (Q10 2.25). Initial uptake rates were not affected by ouabain or NaN3, but efflux of intracellular drug was markedly inhibited by NaN3, suggesting an energy-dependent efflux mechanism. A low affinity uptake component was identified with extracellular I >10μM, possibly representing a lower affinity membrane carrier or passive diffusion. Growth of MCF-7 cells in serum-free medium induced an increase in Km to 15.93μM; insulin, but not estradiol, reversed this change. Thus, I transport in this human solid tumor is similar to that in human leukemia cells.
IT **1225-58-7**
RL: BIOL (Biological study)
(methotrexate transport by breast cancer cells response to)
RN 1225-58-7 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, (16β)- (9CI) (CA INDEX NAME)

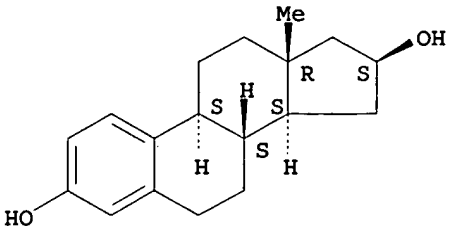
Absolute stereochemistry.



CC 1-2 (Pharmacodynamics)
IT **1225-58-7** 9004-10-8, biological studies
RL: BIOL (Biological study)
(methotrexate transport by breast cancer cells response to)

L52 ANSWER 9 OF 24 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1978:116912 HCAPLUS
DOCUMENT NUMBER: 88:116912
TITLE: Inhibition of human placental 17β-hydroxysteroid dehydrogenase by steroids and nonsteroidal alcohols: aspects of inhibitor structure and binding specificity
AUTHOR(S): Blomquist, Charles H.; Kotts, Claire E.; Hakanson, Erick Y.
CORPORATE SOURCE: Dep. Obstet. Gynecol., St. Paul-Ramsey Hosp., St. Paul, MN, USA
SOURCE: Archives of Biochemistry and Biophysics (1978), 186(1), 35-41
CODEN: ABBIA4; ISSN: 0003-9861
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Inhibition of human placental 17β-hydroxysteroid dehydrogenase by C18 and C19 steroids and nonsteroidal alcs. was assayed at pH 9.0 with 17β-estradiol 3-Me ether and NAD as reactants. The nonsteroidal alcs. tested were poor inhibitors. Cyclopentanol and cyclohexanol had Ki values >5mM. Nonarom. C18 and C19 steroids with O functions at both positions 3 and 17 gave no detectable inhibition or had Ki values ≥160 μm. 3β-Hydroxy-5,16-androstadiene, 5-androsten-3β-ol, 1,3,5(10)-estratrien-3-ol, and 1,3,5(10),16-estratetraen-3-ol, steroids lacking a C(17) oxygen function, had Ki values of 1.8, 6.0, 0.04, and 0.17 μM, resp., demonstrating that both C18 and C19 steroids can bind at the steroid site. Binding specificity is narrowed and binding affinity for nonarom. steroids weakened by O functions at C(17) or both C(3) and C(17). The structural implications of the specificity data for steroid recognition and complex formation and in vivo control of enzyme activity are discussed.
IT **1225-58-7**
RL: BIOL (Biological study)
(17β-hydroxysteroid dehydrogenase inhibition by, kinetics of)
RN 1225-58-7 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, (16β)- (9CI) (CA INDEX NAME)

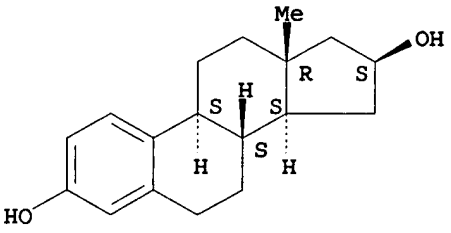
Absolute stereochemistry.



CC 7-3 (Enzymes)
IT 50-27-1 53-16-7, biological studies 53-43-0 53-63-4 57-91-0 58-22-0 63-05-8 96-41-3 100-51-6, biological studies 108-93-0, biological studies 108-95-2, biological studies 112-47-0 547-81-9 1150-90-9 1224-94-8 **1225-58-7** 1476-64-8 1912-63-6 3646-28-4 3937-56-2 5088-64-2 54200-08-7
RL: BIOL (Biological study)
(17β-hydroxysteroid dehydrogenase inhibition by, kinetics of)

L52 ANSWER 10 OF 24 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1973:505459 HCAPLUS
DOCUMENT NUMBER: 79:105459
TITLE: Chromogenic reactions of steroids with strong acids. IV. Specificity of the Kober reaction
AUTHOR(S): Kimura, Michiya; Kawata, Meiji; Akiyama, Kazuyuki; Harita, Kazuaki; Miura, Toshiaki
CORPORATE SOURCE: Fac. Pharm. Sci., Hokkaido Univ., Sapporo, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (1973), 21(8), 1720-6
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The structural requirements were investigated for the Kober reaction of steroidal mols. On the basis of the data given by 94 phenolic steroids and related substance, a compound will give the pos. Kober reaction when a steroidal ring system, a phenolic ring A, double bond or O function in ring D, an angular Me group at C-13, and an angular H atom are present in its mol.
IT **1225-58-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(Kober reaction of, absorption spectra and)
RN 1225-58-7 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, (16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

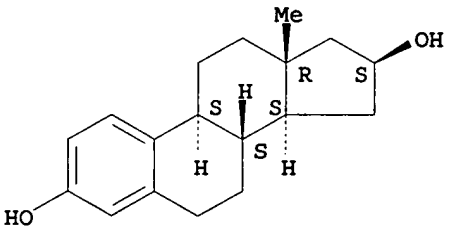


CC 32-3 (Steroids)
Section cross-reference(s): 22
IT 50-23-7 50-24-8 53-41-8 53-42-9 53-45-2 57-83-0,

reactions 57-88-5, reactions 58-22-0 72-33-3 145-13-1
362-06-1 362-07-2 434-22-0 481-29-8 482-49-5 514-61-4
517-07-7 517-09-9 521-10-8 521-11-9 521-17-5 566-75-6
604-82-0 846-46-8 901-93-9 960-28-1 966-47-2 1078-19-9
1089-80-1 1217-09-0 **1225-58-7** 1228-73-5 1232-80-0
1239-35-6 1616-20-2 1730-48-9 2208-13-1 2259-89-4
3601-97-6 4011-48-7 4147-12-0 4954-14-7 5764-23-8
5976-64-7 5976-65-8 5976-68-1 5976-70-5 5982-51-4
6714-06-3 7291-41-0 10323-17-8 13251-78-0 14550-57-3
15236-73-4 15292-90-7 16127-98-3 19518-61-7 26584-88-3
26584-89-4 26584-90-7 28336-31-4 31019-01-9 35456-73-6
40822-17-1 50394-23-5 50394-95-1 50395-01-2 50395-07-8
50395-10-3 50395-12-5 50395-16-9 50395-18-1 50395-21-6
50395-26-1 50395-28-3 50395-30-7 50395-31-8 50395-34-1
50395-35-2 50395-38-5 50770-19-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(Kober reaction of, absorption spectra and)

L52 ANSWER 11 OF 24 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1970:495274 HCAPLUS
DOCUMENT NUMBER: 73:95274
TITLE: Absorption and fluorescence spectra of phenolic steroids and their Kober chromophore
AUTHOR(S): De Lauzon, Solange
CORPORATE SOURCE: Lab. Chim. Biol., Fac. Med., Paris, Fr.
SOURCE: Bulletin de la Societe de Chimie Biologique (1970), 52(2), 181-209
CODEN: BSCIA3; ISSN: 0037-9042
DOCUMENT TYPE: Journal
LANGUAGE: French
AB A complete assignment was made of the absorption and fluorescence spectra of a number of phenolic steroids and their derivs. and the results may be used to identify and determine each estrogen studied. The reaction of various derivs. which cannot be differentiated by the behavior of the Kober chromophore, or do not form a Kober chromophore, in H2SO4 and H3PO4 was used as an identification method. These derivs. included ketonic derivs. of estrone and estradiol, 16-hydroxy derivs. of estrone and their Et and Me ethers, and non-oxygenated C17 derivs. The Kober reaction was used as a determination method for derivs. giving a characteristic absorption maximum, and the Ittrich modification allowed a sensitive anal. method to be developed for the steroid groups.
IT **1225-58-7**
RL: PRP (Properties)
(fluorescence and visible spectra of, and its Kober chromogen)
RN 1225-58-7 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, (16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

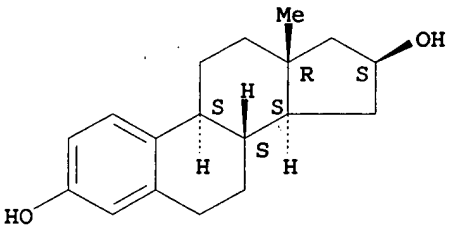


CC 6 (Biochemical Methods)
IT 50-27-1 50-28-2, properties 53-16-7, properties 57-91-0
362-07-2 362-08-3 547-81-9 566-75-6 566-76-7 571-92-6
793-89-5 966-06-3 1035-77-4 1090-04-6 **1225-58-7**

1228-72-4 1228-73-5 1229-33-0 1474-50-6 1474-53-9
1476-34-2 1624-62-0 3434-76-2 3434-77-3 3434-78-4
3434-79-5 3434-81-9 5976-64-7 6038-22-8 7004-98-0
24721-15-1 26849-20-7 28872-65-3
RL: PRP (Properties)
(fluorescence and visible spectra of, and its Kober chromogen)

L52 ANSWER 12 OF 24 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1970:452631 HCAPLUS
DOCUMENT NUMBER: 73:52631
TITLE: Steroid utilization by amphibian skin
AUTHOR(S): Ferguson, M. M.; McGadey, J.
CORPORATE SOURCE: Anat. Dep., Univ. Glasgow, Glasgow, UK
SOURCE: Histochemie (1970), 22(1), 36-8
CODEN: HICHAU; ISSN: 0018-2222
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The glands which secrete unpleasant tasting or toxic substances in amphibian dermis were investigated histochem. for hydroxysteroid dehydrogenase (I) activity to draw comparisons with mammalian sebaceous glands, which are known to utilize hydroxy steroids. Skin sections from frogs were incubated with 15 different steroids; serial sections were also stained with hematoxylin and eosin and by the periodic acid-Schiff (PAS) reaction to differentiate mucous glands. The frog skin contained at least 2 functional types of glands; one type was PAS-pos., while the second type, less common, was PAS-neg. but exhibited intense I activity. Tissue incubated with pregnenolone, dehydroepiandrosterone, 3β-hydroxyandrost-5-en-16-one 3-methyl ether, and 2β-hydroxyprogesterone exhibited no formazan deposits.
IT **1225-58-7**
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(metabolism of, by skin)
RN 1225-58-7 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, (16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 4 (Hormones and Related Substances)
IT 50-23-7, biological studies 50-28-2, biological studies 53-06-5, biological studies 53-41-8 53-42-9 53-43-0, biological studies 58-22-0, biological studies 145-13-1 145-15-3 481-29-8 571-31-3 **1225-58-7** 5888-04-0 6038-34-2
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(metabolism of, by skin)

L52 ANSWER 13 OF 24 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1965:10380 HCAPLUS
DOCUMENT NUMBER: 62:10380
ORIGINAL REFERENCE NO.: 62:1938e-f

TITLE: A search for inhibitors of prostate growth stimulators
AUTHOR(S): Tesar, Charles; Scott, William Wallace
CORPORATE SOURCE: Johns Hopkins Hosp., Baltimore, MD, USA
SOURCE: Investigative Urology (1964), 1(5), 482-98
CODEN: INURAQ; ISSN: 0021-0005
DOCUMENT TYPE: Journal
LANGUAGE: English

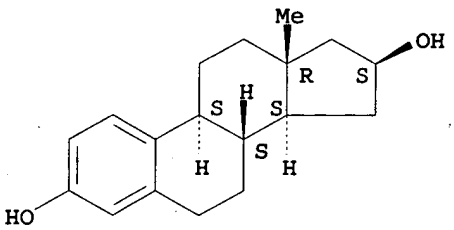
AB Wistar rats received 0.4 mg. testosterone propionate (I) s.c. every other day for 8 days following castration. Test compds. were given at 0.5, 1, and 2 mg. every other day for 7 days, with or without 0.4 mg. I in castrate and noncastrates, resp. Within 48 h. of the 7th (final) injection, animals were sacrificed with CHCl3, and the prostate weight to body weight ratio, and the prostate weight index were determined The greatest prostate growth inhibitor was 17β-estradiol, and some weak inhibition was seen with 6α-methyl-4-pregnene-3,20-dione-17α-ol acetate, androstane-3,17-dione, and 2α-methyl-4-estrene-17β-ol-3-one, the inhibitory effect being seen only in intact rats, and not in castrates, for all 52 compds. tested.

IT **1225-58-7**, Estra-1,3,5(10)-triene-3,16β-diol
(as prostate growth inhibitor)

RN 1225-58-7 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



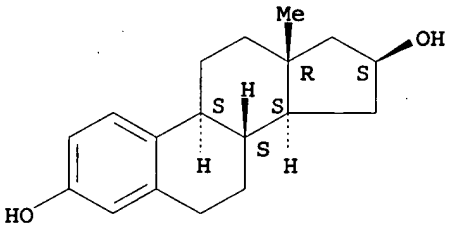
CC 58 (Hormones)

IT 57-91-0, 17α-Estradiol 65-14-5, Valeronitrile, 2,3-bis(p-hydroxyphenyl)- 68-22-4, 19-Nor-17α-pregn-4-en-20-yn-3-one, 17-hydroxy- 68-96-2, Pregn-4-ene-3,20-dione, 17-hydroxy- 71-58-9, Pregn-4-ene-3,20-dione, 17-hydroxy-6α-methyl-, acetate 521-12-0, 5α-Androstan-3-one, 17β-hydroxy-2α-methyl-, propionate 571-22-2, 5β-Androstan-3-one, 17β-hydroxy- 1039-17-4, Androsta-4,9(11)-dien-3-one, 17β-hydroxy-17-methyl- 1090-04-6, Estra-1,3,5(10)-triene-3,16α-diol 1092-04-2, Estr-4-en-3-one, 17β-hydroxy-2α-methyl- 1093-46-5, 19-Nor-17α-pregn-20-yne-3β,17-diol 1094-07-1, Estra-1,3,5(10-trien-17-one, 3-hydroxy-1,2-dimethyl- 1096-38-4, Pregna-4,16-diene-3,20-dione **1225-58-7**, Estra-1,3,5(10)-triene-3,16β-diol 1229-33-0, Estra-1,3,5(10)-trien-16β-ol, 3-methoxy- 1428-66-6, Acetic acid, [(17-oxoestra-1,3,5(10)-trien-3-yl)oxy]- 1428-67-7, Propionitrile, 2,3-bis(p-hydroxyphenyl)- 5717-79-3, 5α-Androstane-3,17-dione, 17-oxime 6808-29-3, 19-Nor-17α-pregn-20-yn-3-one, 17-hydroxy-
(as prostate growth inhibitor)

L52 ANSWER 14 OF 24 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1960:98911 HCAPLUS
DOCUMENT NUMBER: 54:98911
ORIGINAL REFERENCE NO.: 54:18799c-d
TITLE: Cytostatic activities of steroidal estrogens

against zebra-fish embryos
AUTHOR(S): Jones, Roy W.; Rhone, James R.; Huffman, Max N.
CORPORATE SOURCE: Oklahoma State Univ., Stillwater
SOURCE: Proceedings of the Society for Experimental Biology and Medicine (1960), 104, 190-1
CODEN: PSEBAA; ISSN: 0037-9727
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB cf. CA 52, 3171c. The cytostatic effects of 14 steroidal estrogens (named) and the 3-Me and 3-Et ethers of each were tested on embryos of zebra-fish (Brachydanio rerio) as test object. Many were inactive in the concns. used. Most active was 17-dihydro-17 β-equilin 3-ethyl ether (effective at 0.5 p.p.m.). There was no relation whatever between estrogenic hormone potency and cytostatic potency.
IT **1225-58-7**, Estra-1,3,5(10)(triene-3,16β-diol
(as cell-division inhibitor)
RN 1225-58-7 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, (16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 11I (Biological Chemistry: Zoology)
IT 50-28-2, Estradiol 57-91-0, 17α-Estradiol 517-09-9, Equilenin 1035-77-4, Estra-1,3,5(10)-trien-17β-ol, 3-mehoxy- 1090-04-6, Estra-1,3,5(10)-triene-3,16α-diol **1225-58-7**, Estra-1,3,5(10)(triene-3,16β-diol 1229-33-0, Estra-1,3,5(10)-trien-16β-ol, 3-methoxy- 1423-97-8, Estra-1,3,5(10),6,8-pentaene-3,17β-diol 1474-50-6, Estra-1,3,5(10)-trien-17-one, 3-ethoxy- 1624-62-0, Estra-1,3,5(10)-trien-17-one, 3-methoxy- 3494-09-5, Estra-1,3,5(10)-trien-17β-ol, 3-ethoxy- 3563-27-7, Estra-1,3,5(10),7-tetraene-3,17β-diol 4820-55-7, Estra-1,3,5(10),6,8-pentaen-17β-ol, 3-methoxy- 6030-83-7, Estra-1,3,5(10),7-tetraen-17-one, 3-methoxy- 6038-22-8, Estra-1,3,5(10)-trien-16-one, 3-methoxy- 13587-68-3, Estra-1,3,5(10),7-tetraen-17β-ol, 3-methoxy- 58031-57-5, Estra-1,3,5(10),6,8-pentaen-17β-ol, 3-ethoxy- 102168-54-7, Estra-1,3,5(10)-triene-16,17-dione, 3-ethoxy- 110145-73-8, Estra-1,3,5(10),7-tetraen-17-one, 3-ethoxy- 110876-82-9, Estra-1,3,5(10),7-tetraen-17β-ol, 3-ethoxy- 112949-05-0, Estra-1,3,5(10)-trien-16β-ol, 3-ethoxy-
(as cell-division inhibitor)

L52 ANSWER 15 OF 24 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1960:74827 HCAPLUS
DOCUMENT NUMBER: 54:74827
ORIGINAL REFERENCE NO.: 54:14309a-e
TITLE: 16α-Hydroxysteroids
PATENT ASSIGNEE(S): Nepera Chemical Co., Inc.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 823955		19591118	GB 1956-11714	19560417

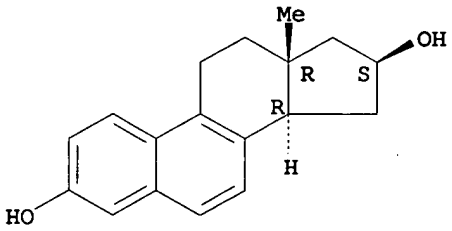
AB The title compds., their ethers and esters were prepared by heating an arenesulfonate of the corresponding 16β-ol with an alkali metal lower alkanoate in the corresponding alkanoic acid and saponifying the resulting 16α-acylate. Thus, 4.4 g. p-MeC6H4SO2Cl added to a solution of 1 g. 1,3,5(10)-estratriene-3,16β-diol in 28 ml. dry C5H5N at 0°, the mixture kept 2 days, diluted with ice H2O containing 10% NaCl, left 24 hrs. at 5°, extracted with Et2O, the exts. washed, the washings extracted with Et2O and the combined exts. evaporated gave 1.9 g. crude 3,16β-ditosylate, which refluxed 1 hr. with 4.8 g. fused NaOAc in 92 ml. AcOH, the mixture cooled and diluted with ice H2O containing 10% NaCl, after 24 hrs. the precipitate separated, dried and refluxed 1 hr. with 60 ml. 2.5N KOH in 200 ml. MeOH, the MeOH distilled, 100 ml. H2O, then 10 ml. concentrated HCl added, the pH adjusted to 5-6, the precipitate separated, dried at 40° and crystallized from Me2CO-hexane then aqueous MeOH gave 0.55 g. 3,16α-estradiol (I), m. 213-15°, raised to 224-4.5°, [α]25D 85° (c 0.76, 95% EtOH), after purification via its 3,16α-diacetate, m. 116-17°. Benzoylation of I in 0.5N NaOH gave the 3-monobenzoate, m. 179.5-81.0°; benzoylation in C5H5N gave the 3,16-dibenzoate, m. 130.5-1.5°. Similarly, 118 mg. 3-methoxyestra-1,3,5(10)-trien-16β-ol gave 38 mg. estradiol 16α-acetate 3-methyl ether, m. 123-3.5°; 575 mg. androstan-3β-ol-16-one dissolved in 300 ml. refluxing MeOH, cooled, 0.39 g. NaBH4 added, the solution swirled 1 hr., 4 ml. 50% AcOH added, the solution concentrated to 100 ml. and 100 ml. ice H2O added yielded 550 mg. 3β-benzoyloxyandrostan-16β-ol (II), m. 168-9°; 400 mg. II epimerized as above gave androstane-3β,16α-diol, m. 187.5-88°, [α]25D -4° (c 0.777, 95% EtOH), which with Ac2O in C5H5N gave the diacetate, m. 174-4.5° [α]23D -26° (c 0.963, CHCl3). Other starting materials are equilenin-16-one and 5-isoandrosterone. I displays considerable estrogenic activity, in contrast to its 16β epimer.

IT **110012-46-9**, Estra-1,3,5(10),6,8-pentaene-3,16β-diol (isomerization of)

RN 110012-46-9 HCAPLUS

CN Estra-1,3,5(10),6,8-pentaene-3,16-diol, (16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 10J (Organic Chemistry: Steroids)

IT 109581-80-8, Estra-1,3,5(10),7-tetraene-3,16β-diol
110012-46-9, Estra-1,3,5(10),6,8-pentaene-3,16β-diol (isomerization of)

L52 ANSWER 16 OF 24 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1959:17432 HCAPLUS
DOCUMENT NUMBER: 53:17432
ORIGINAL REFERENCE NO.: 53:3276g-i,3277a-f
TITLE: Synthesis of 1,3,5(10)-estratriene-3,16β,17α-triol
AUTHOR(S): Fishman, Jack; Biggerstaff, Warren R.
CORPORATE SOURCE: Sloan-Kettering Inst. for Cancer Research, New York, NY
SOURCE: Journal of Organic Chemistry (1958), 23, 1190-2
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 53:17432

AB Preparation of 1,3,5(10)-estratriene-3,16β,17α-triol (I) is described. The 16α- (II) and 16α-bromo epimers (III) of estrone were also prepared and some of their reactions studied. Of the 4 possible estriols isomeric at C-16 and C-17 only 3 are known. The present authors undertook the preparation of the remaining isomer, I. Estrone enol diacetate (1 g.) in CCl4 containing some K2CO3 was treated with 1 equivalent of Br in CCl4 and the mixture worked up to give 700 mg. 16α-bromoestrone acetate (IV), m. 169-71° (MeOH), [α]24D 119° (CHCl3). IV (0.3 g.) in 4% alc. H2SO4 left 20 hrs. at room temperature, diluted with H2O, and extracted with CHCl3 gave 243 mg. II, needles, m. 225-8° (C6H6), [α]24D 120° (CHCl3). Acetylation of II with Ac2O and C5H5N regenerated IV. IV (0.5 g.) in a min. amount of 1:1 C6H6-ligroine was absorbed on Al2O3, left overnight on the column and eluted with first 3:2 and then 4:1 C6H6-ligroine, and the fractions combined on the basis of m.p. The first 5 fractions gave on crystallization 0.23 g. pure IV. Fractions 6-10 were mixts., and fractions 10-14 gave 47 mg. 16β-bromoestrone acetate (V), needles, m. 170-3° (MeOH), [α]25D 156° (CHCl3). Subsequent fractions eluted from the column with more polar solvents proved to be a mixture of the hydrolyzed II and III. A mixed m.p. of V with IV showed a depression of 40°; the infrared spectra of II and III in CS2 were different in the 1400-650 cm.-1, but there was no difference in the position of the CO band at 1758 cm.-1 Paper chromatography in several systems failed to sep. the 2 isomers. Room temperature hydrolysis of V 20 hrs. with 4% alc. H2SO4 gave free III, needles, m. 224-7° (sublimation) (C6H6). An analytical sample of III m. 225-8°, [α]24D 154° (CHCl3). III could be obtained by refluxing IV with 4% alc. H2SO4 overnight; the resultant mixture was predominantly III which was purified by fractional crystallization Acetylation of III gave V. IV (1 g.) stirred 2 hrs. at 0° with excess LiAlH4 in anhydrous Et2O, the excess reagent destroyed with H2O and acidified with dilute HCl, and the organic phase evaporated gave 0.78 g. gum. Without purification, the material refluxed 4 hrs. with 5% alc. KOH, diluted with H2O, extracted with CHCl3, and chromatographed on Al2O3 gave 0.24 g. 16β,17β-epoxy-1,3,5(10)-estratrien-3-ol (VI), m. 200-4° (C6H6-ligroine), [α]25D 119° (CHCl3), and 92 mg. estrone. The structure of VI was established by reduction with LiAlH4 to give 16β-estradiol (VII), identical with a specimen prepared from 1,3,5(10)-estratrien-16-one by NaBH4 reduction. VII m. 224-6°. V (150 mg.) reduced under identical conditions with LiAlH4 followed by heating with alkali gave 94 mg. estrone. No 16α,17α-oxide was isolated. VI (0.3 g.) in 30 cc. AcOH refluxed 4 hrs., evaporated, refluxed 1.5 hrs. with 6% alc. KOH, diluted, acidified, and extracted with CHCl3 gave 0.3 g. solid which was chromatographed on Al2O3 to give 124 mg. I, m. 248-50° (C6H6-MeOH), [α]25D 61° (alc.). The subsequent fractions eluted weighed 64 mg. and proved to be

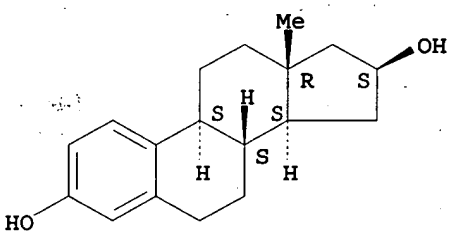
the other trans isomer, 1,3,5(10)-estratriene-3,16β,17α-triol (VIII). The infrared spectrum of I in KBr showed differences from the other 3 estriol isomers. Paper chromatography in C6H6-MeOH-H2O-EtOAc system separated I from its isomers. I was less polar than VIII but considerably more polar than the 2 cis triols in the solvent system used. 1,3,5(10),16-Estratetraen-3-ol benzoate (100 mg.), m. 161-6°, in Et2O treated with BzO2H gave 111 mg. crude 16α,17α-epoxy-1,3,5(10)-estratrien-3-ol benzoate. Without further purification this material was refluxed 2 hrs. with 3 cc. AcOH under N, the AcOH removed, and the residue refluxed 1.5 hrs. in 8% alc. KOH to give 73 mg. yellow solid, which, decolorized and crystallized, gave 23 mg. solid which was chromatographed on silica to give 12 mg. I. These results confirm the assignment of the Br orientation in II and III and also support the previous finding (C.A. 52, 5445b) that a 16β-substituent results in the stereospecific β-reduction of the 17-one while a 16α-substituent makes the reduction only stereoselective, with about 10-15% of α-reduction. The pharmacol. effects are being investigated.

IT **1225-58-7**, Estra-1,3,5(10)(triene-3,16β-diol
(preparation of)

RN 1225-58-7 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 10J (Organic Chemistry: Steroids)

IT 50-27-1, Estriol 472-57-1, Estra-1,3,5(10)-trien-3-ol, 16β,17β-epoxy- 793-89-5, Estra-1,3,5(10)-triene-3,16β,17α-triol **1225-58-7**, Estra-1,3,5(10)(triene-3,16β-diol 1228-71-3, Estrone, 16β-bromo- 1239-35-6, Estrone, 16α-bromo-, acetates 65912-80-3, Estrone, 16β-bromo-, acetates 71765-95-2, Estrone, 16α-bromo- 114277-40-6, Estra-1,3,5(10)-trien-3-ol, 16α,17α-epoxy-, benzoate
(preparation of)

L52 ANSWER 17 OF 24 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1958:93818 HCAPLUS

DOCUMENT NUMBER: 52:93818

ORIGINAL REFERENCE NO.: 52:16548d-f

TITLE: Comparative ability of some steroids and their esters to enhance the renal β-glucuronidase activity of mice

AUTHOR(S): Fishman, Wm. H.; Lipkind, J. B.

CORPORATE SOURCE: Tufts Univ. School of Med., Boston, MA

SOURCE: Journal of Biological Chemistry (1958), 232, 729-36
CODEN: JBCHA3; ISSN: 0021-9258

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB cf. C.A. 50, 17081h. The mouse renal β-glucuronidase response permits a more reliable estimate of the potency of

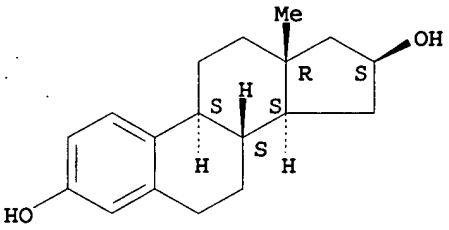
testosterone esters. A dose-response curve in which greatly reduced amts. of steroid were used was employed. The potency of a steroid in eliciting the β-glucuronidase response is defined as 24 times the reciprocal of the dose required to produce a kidney assaying 10,000 units/g. The standard of reference is testosterone. According to this measure, testosterone propionate shows a potency of 60 and that of testosterone is 3.0. Nortestosterone cyclopentylpropionate was the most potent compound (potency 150). There is a marked difference in response between testosterone propionate and its other esters vs. testosterone. 3,16β-Estradiol and 16-oxoestrone gave 2- to 3-fold increases in renal β-glucuronidase. The introduction of a 17-Me or 17-Et group into nortestosterone increased its potency as determined by the renal β-glucuronidase response.

IT **1225-58-7**, Estra-1,3,5(10)(triene-3,16β-diol
(potentiation of β-glucuronidase of kidneys by)

RN 1225-58-7 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 11F (Biological Chemistry: Physiology)

IT 601-63-8, Estr-4-en-3-one, 17β-hydroxy-, cyclopentanepropionate **1225-58-7**, Estra-1,3,5(10)(triene-3,16β-diol 1228-73-5, Estra-1,3,5(10)-triene-16,17-dione, 3-hydroxy- 100151-63-1, Estr-4-en-3-one, 17β-hydroxymethyl-
(potentiation of β-glucuronidase of kidneys by)

L52 ANSWER 18 OF 24 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1957:101244 HCAPLUS

DOCUMENT NUMBER: 51:101244

ORIGINAL REFERENCE NO.: 51:18311d-g

TITLE: The effect of natural and synthetic estrogens on reticuloendothelial system function

AUTHOR(S): Heller, J. H.; Meier, R. M.; Zucker, R.; Mast, G. W.

CORPORATE SOURCE: New England Inst. for Med. Research, Ridgefield, CT

SOURCE: Endocrinology (1957), 61, 235-41

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB The activity of the reticuloendothelial system was determined by measuring the rate of disappearance by phagocytosis of intravenously injected colloidal C from the blood. The colloid uptake of various organs was determined by assaying for CrP3204 content after an intravenous injection. Steroids increasing phagocytic velocity 100% or more were: estradiol, ethynylestradiol, estradiol-16-one, 1,3,5-estratriene-3,16β-diol, 3-methoxy-1,3,5-estratriene-16β-ol, estriol, 16-epiestriol, 3-methoxy-1,3,5-estratriene-16β,17β-diol, and 3-ethoxy-1,3,5-estratriene-16β,17β-diol; inactive were: 5-androstene-3β,16β-diol, androstane-3,16β-diol, androstane-3α-ol-16-one, 4-androstene-3,16-dione, 5-androstene-3β-ol-16-one, 3β-methoxy-5-androstene-16-

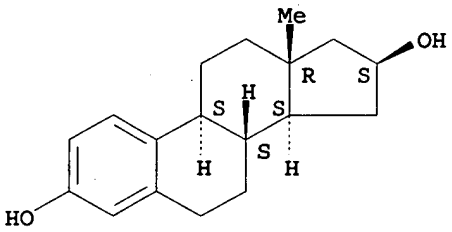
one, 1,3,5-estratriene-3,6α-diol, and 3-methoxy-1,3,5-estratriene-16-one. Stimulated activity of the reticuloendothelial system was accompanied by liver and spleen enlargement, without however, much increase in total colloid uptake by these organs.

IT **1225-58-7**, Estra-1,3,5(10)(triene-3,16β-diol
(effect on reticuloendothelial system)

RN 1225-58-7 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 11H (Biological Chemistry: Pharmacology)

IT 566-75-6, Estra-1,3,5(10)-trien-16-one, 3,17β-dihydroxy-
1225-58-7, Estra-1,3,5(10)(triene-3,16β-diol
1229-33-0, Estra-1,3,5(10)-trien-16β-ol, 3-methoxy-
3434-79-5, Estra-1,3,5(10)-triene-16β,17β-diol, 3-methoxy- 26849-20-7, Estra-1,3,5(10)-triene-16β,17β-diol, 3-ethoxy-
(effect on reticuloendothelial system)

L52 ANSWER 19 OF 24 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1957:47334 HCAPLUS

DOCUMENT NUMBER: 51:47334

ORIGINAL REFERENCE NO.: 51:8819i,8820a-h

TITLE: 3,16α-Steroid diols

INVENTOR(S): Huffman, Max N.

PATENT ASSIGNEE(S): Nepera Chemical Co., Inc.

DOCUMENT TYPE: Patent

LANGUAGE: Unavailable

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2779773		19570129	US 1956-586637	1956 0523

OTHER SOURCE(S): CASREACT 51:47334

AB Estrogen and androgen steroids diols with 16α-configuration and the corresponding ether and ester derivs. have considerable physiol. activity in comparison with their β-isomers. 1,3,5(10)-Estratriene-3,16β-diol (1 g.) in 28 ml. dry pyridine at 0° treated with 4.4 g. p-MeC6H4SO2Cl, the mixture kept 2 days at room temperature, diluted with ice H2O containing 10% NaCl, the mixture kept 24 hrs. at 5°, extracted with Et2O, and the washed and dried extract evaporated on a steam bath gave 1.9 g. crude ditosylate, which treated with 4.8 g. freshly fused NaOEt and 92 ml. AcOH, the mixture refluxed 1 hr. at 138-50°, cooled to 5°, treated 24 hrs. with ice H2O containing 10% NaCl, filtered, the dried residue saponified by refluxing 1 hr. with 200 ml. MeOH and 60 ml. 2.5N KOH, the MeOH evaporated, 100 ml. H2O added, the clear solution treated with 10 ml. concentrated HCl and the pH adjusted to 5-6

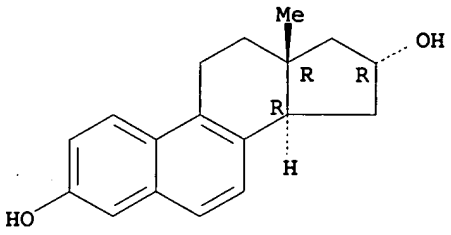
with AcOH, filtered, and the dried product (0.88 g.) recrystd. from C6H14 and aqueous MeOH gave crude 3,16α-estradiol (I), m. 213-15°, purified through the diacetate, m. 116-17°, to pure I, m. 224.0-4.5°, [α]D25 85° (c 0.76%, 95% alc.). Similarly were prepared 1,3,5(10),6,8-estrapentaene-3,16α-diol (II) and 1,3,5(10),7-estratetraene-3,16α-diol (III). Alkylation of II and III gave the corresponding diacetates and dipropionates. I (46 mg.) in 30 ml. 0.5N NaOH stirred with 0.5 ml. BzCl, the mixture kept overnight at room temperature, filtered, the washed residue dried in vacuo and recrystd. from Me2CO-C6H14 and aqueous MeOH gave 3-benzoxy-1,3,5(10)-estratrien-16α-ol, m. 179.5-181.0°. I (150 mg.) in 6.0 ml. dry pyridine stirred 24 hrs. with 1.5 ml. BzCl, the mixture poured into ice H2O, the oily product crystallized from alc. Me2CO containing a trace of pyridine, and repeatedly recrystd. from Me2CO-C6H14 and 95% alc. yielded 132 mg. 1,3,5(10)-estratriene-3,16α-diol dibenzoate, m. 130.5-1.5°. The dipropionate, dibutyrate, divalerate, dipalmitate, distearate, bis(phenylacetate), dinaphthoate, bis(cyclopentylpropionate), and ditoluate were similarly prepared Treatment of 118 mg. 3-methoxy-1,3,5(10)-estratrien-16α-ol in 2 ml. pyridine with 0.2 g. p-MeC6H4SO3Cl gave the corresponding 16-p-toluenesulfonate, converted by heating 1 hr. with 200 mg. fused NaOAc and 4.0 ml. AcOH to 3,16α-estradiol 3-Me ether; 16α-acetate, m. 123.0-3.5°. 3β-Androstanol-16-one benzoate (575 mg.) in 300 ml. MeOH was stirred 1 hr. at room temperature with 0.39 g. NaBH, the mixture treated slowly with 4 ml. 50% AcOH, concentrated to 100 ml. at 100°, cooled with 100 ml. ice water and the product crystallized by standing 2 days at 0° to give 550 mg. 3β,16β-androstanediol 3-benzoate (IV), m. 168-9°. IV (400 mg.) in 8 ml. dry pyridine treated with 0.8 g. p-MeC6H4SO2Cl, the mixture poured into ice water, filtered, the residue dried in vacuo, refluxed 1 hr. with 1 g. fused NaOAc and 20 ml. AcOH at 137-53°, the cooled mixture extracted with Et2O, the washed and dried extract evaporated, the residue saponified 24 hrs. in 7.5 g. KOH, 12.5 ml. H2O, and 100 ml. MeOH, the free diol extracted with Et2O, the washed and dried extracted evaporated, and the residue purified by repeated recrystn. from Me2CO-C6H14, MeCOEt-C7H16 and Me2CO-C6H4 yielded 3β,16α-androstanediol (V), m. 187.5-8.0°, [α]D25 -4° (c 0.777, 95% alc.); diacetate, m. 174.0-4.5°, [α]D23 -26° (c 0.963, CHCl3). Similarly 5-androsten-3β-ol-one benzoate or etiocholan-3α-ol-16-one benzoate can be transformed to the corresponding 16β-diol and epimerized to the 16α-diol. I (38 mg.) in 8 ml. 90% MeOH and 0.8 g. K2CO3 refluxed, the mixture treated with 0.3 ml. Me2SO4, refluxed after the reaction with addnl. 0.3 ml. Me2SO4, the mixture distilled with 4 ml. H2O, the turbid mixture filtered, the product washed with H2O and dried in vacuo, taken up in Me2CO and the solution evaporated gave 3,16α-estradiol 3-Me ether. Other 3-ethers are similarly prepared and ether groups may be formed at the 16-HO group by use of twice the amount of dialkyl sulfates.

IT **109932-04-9**, Estra-1,3,5(10),6,8-pentaene-3,16α-diol (esters)

RN 109932-04-9 HCAPLUS

CN Estra-1,3,5(10),6,8-pentaene-3,16-diol, (16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



(prepn. of
CC 10 (Organic Chemistry)
IT 1090-04-6, Estra-1,3,5(10)-triene-3,16α-diol 109396-95-4, Estra-1,3,5(10),7-tetraene-3,16α-diol **109932-04-9**, Estra-1,3,5(10),6,8-pentaene-3,16α-diol
(esters)
IT 22630-49-5, 5α-Androstane-3β,16α-diol
54657-07-7, 5α-Androstane-3β,16α-diol, diacetate
74111-56-1, Estra-1,3,5(10)-trien-16α-ol, 3-methoxy-
76820-87-6, Estra-1,3,5(10)-trien-16α-ol, 3-methoxy-, acetate 109396-95-4, Estra-1,3,5(10),7-tetraene-3,16α-diol
109932-04-9, Estra-1,3,5(10),6,8-pentaene-3,16α-diol
115484-92-9, 5α-Androstane-3β,16β-diol, 3-benzoate
(preparation of)

L52 ANSWER 20 OF 24 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1956:48821 HCAPLUS
DOCUMENT NUMBER: 50:48821
ORIGINAL REFERENCE NO.: 50:9438h-i,9439a-c
TITLE: 16-Substituted steroids. XIV. A new synthetic route to Δ16-steroids
AUTHOR(S): Huffman, Max N.; Lott, Mary Harriet; Tillotson, Albert
CORPORATE SOURCE: Oklahoma Med. Research Foundation, Oklahoma City
SOURCE: Journal of Biological Chemistry (1955), 217, 103-6
CODEN: JBCHA3; ISSN: 0021-9258
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 50:48821
AB cf. C.A. 50, 4178c. A new preparative method for ring D-substituted Δ16-steroids is described; it involves collidine cleavage of the 16-p-toluenesulfonate to effect a double bond at C-16-C-17. This synthetic route may have wide usefulness in the steroid field. 1,3,5(10)-Estratriene-3,16β-diol (1.00 g.) in 500 cc. 0.7N KOH at 15° shaken 10 min. with 8 cc. BzCl, the mixture held overnight at room temperature, filtered, the benzoate refluxed in 150 cc. EtOH containing 0.1 cc. pyridine and 0.1 cc. AcOH, diluted with 25 cc. water, filtered, and the filtrate concentrated to crystallization and held 24 hrs. at 5° yielded 1.23 g. 3-benzoxy-1,3,5(10)-estratrien-16β-ol (I), m. 144-5°. I in 30 cc. dry pyridine at 0-5° treated with 3 g. solid p-MeC6H4SO2Cl (II), and the mixture held 1 hr. in the ice bath, then 1 day at room temperature, diluted with 600 cc. ice water, held 1 day at 5°, and filtered yielded 1.53 g. crude tosylate (III). III (1.53 g.) refluxed 4 hrs. with 120 cc. collidine, the cooled mixture shaken with 0.7N H2SO4 and Et2O, and the Et2O phase washed yielded 900 mg. 1,3,5(10), 16-estratetraen-3-ol benzoate (IV), m. 164-7°. IV refluxed 2 hrs. with 400 cc. EtOH containing 16 cc. 2.5N KOH, diluted with 200 cc. water, the alc. removed, the residue partitioned between 600 cc. 1.1% NaHCO3 and 800 cc. C6H6, the C6H6 phase evaporated, and the residue rebenzoylated yielded 570 mg. pure 1,3,5(10),16-estratetraen-3-ol benzoate (V), m. 177-8°,

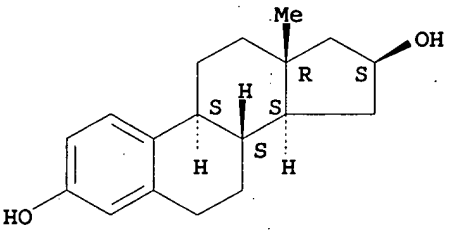
[α]D22 84° (c 0.96, CHCl3). V (390 mg.) refluxed 2 hrs. with 250 cc. MeOH containing 25 cc. N KOH, the mixture diluted with 75 cc. water, the MeOH removed, and the cooled residue neutralized with 1.75 cc. AcOH, held 1 day at 5°, and filtered yielded 120 mg. 1,3,5(10),16-estratetraen-3-ol, m. 130-1.5°, [α]D25 115° (c 1.50, CHCl3); concentration of the filtrate yielded an addnl. 70 mg. m. 128.5-30°.

IT **1225-58-7**, 1,3,5(10)-Estratriene-3,16β-diol (esters)

RN 1225-58-7 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 10 (Organic Chemistry)

IT **1225-58-7**, 1,3,5(10)-Estratriene-3,16β-diol (esters)

L52 ANSWER 21 OF 24 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1956:36437 HCAPLUS

DOCUMENT NUMBER: 50:36437

ORIGINAL REFERENCE NO.: 50:7183a-d

TITLE: Specificity, kinetics, and inhibition of α- and α-hydroxysteroid dehydrogenases

AUTHOR(S): Talalay, Paul; Marcus, Philip I.

CORPORATE SOURCE: Univ. of Chicago

SOURCE: Journal of Biological Chemistry (1956), 218, 675-91
CODEN: JBCHA3; ISSN: 0021-9258

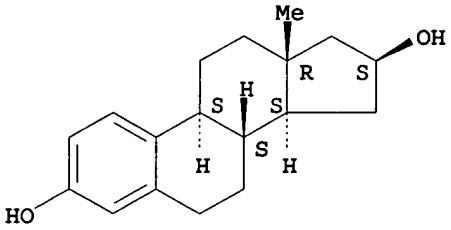
DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB cf. preceding abstract β-Hydroxysteroid dehydrogenase catalyzes the reversible DPN-linked oxidation of 3β-, 16β- and 17β-hydroxy steroids. α-Hydroxysteroid dehydrogenase catalyzes the reversible DPN-linked oxidation of 3 α-hydroxysteroids of the C19, C21, and C24 series. The rates of oxidation of various steroids by these enzymes were determined The pH of the medium affects the equilibrium point and initial velocities of the reactions catalyzed by α- and β-enzymes. The equilibrium constant for the conversion of testosterone to 4-androstene-3,17-dione is 2.6 + 10-8 and that for the conversion of androsterone to androstane-3,17-dione is 5.8 + 10-9. The enzymes can be used for the specific enzymic microassay of selected groupings on the steroid nucleus either singly or in combination. Examples of the determination of 3 α-hydroxyl groups and 3β- and 17β-hydroxyl groups are given and the use of these enzymes for enzymic identification is illustrated. Michaelis consts. of α- and β-enzymes for DPN with various substrates were determined β-Enzyme is strongly inhibited by 3,17β-estradiol and certain related 1,3,5-estratrienes, as well as by diethylstilbestrol and diethylhexestrol. The structural requirements for β-enzyme inhibitions are present.

IT **1225-58-7**, 1,3,5(10)-Estratriene-3,16β-diol
(β-hydroxy steroid dehydrogenase inhibition by)
RN 1225-58-7 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, (16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 11A (Biological Chemistry: General)
IT 50-27-1, Estriol 53-63-4, 1,3,5(10)-Estratrien-3-ol 547-81-9, 1,3,5(10)-Estratriene-3,16β,17β-triol 566-75-6, 1,3,5(10)-Estratrien-16-one, 3,17β-dihydroxy- 1090-04-6, 1,3,5(10)-Estratriene-3,16α-diol **1225-58-7**, 1,3,5(10)-Estratriene-3,16β-diol 2529-64-8, 1,3,5(10)-Estratrien-17β-ol 5635-50-7, Phenol, 4,4'-(1,2-diethylethylene)di- 6898-97-1, 4,4'-Stilbenediol, α,α'-diethyl- 20576-40-3, 1,3,5(10)-Estratrien-17α-ol
(β-hydroxy steroid dehydrogenase inhibition by)

L52 ANSWER 22 OF 24 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1956:28422 HCAPLUS
DOCUMENT NUMBER: 50:28422
ORIGINAL REFERENCE NO.: 50:5784i,5785a-d
TITLE: Estrogenic compounds
INVENTOR(S): Huffman, Max N.
PATENT ASSIGNEE(S): Nepera Chemical Co., Inc.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

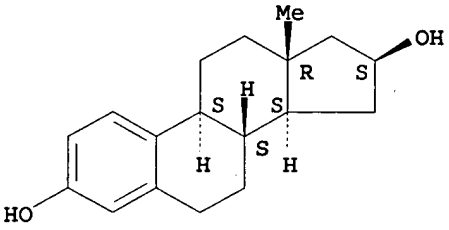
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2705239		19550329	US 1953-354409	1953 0511

AB 16-Estrone (I) (250 mg.) hydrogenated with PtO2 in 0.5N NaOH during 12 hrs. at 25°, then left 24 hrs. at 25°, the mixture acidified, extracted with Et2O, the crystalline residue refluxed 3 hrs. with 0.24 g. HO2CCH2ONH2.0.5HCl, 0.37 g. KOAc, and 40 cc. aqueous PrOH (1:3), left 24 hrs. at 25°, extracted with Et2O, the extract treated with 3% NaHCO3 to remove unchanged material, washed, and the product crystallized yielded 3,16-estradiol (II), m. 224-6° (from Me2CO). A mixture of estrone and I (800 mg.) reduced 30 min. in MeOH with 0.2 g. NaBH4, stirred 0.5 hr., 15 cc. N NaOH added, and the mixture left at room temperature 24 hrs. gave, after a lengthy purification, 154 mg. II. II with NaOH and BzCl in H2O gave the 3-benzoate (III), needles, m. 145-6°, saponified to II. Extremely pure II m. 227-7.5°, [α]D21 79° (95% EtOH). Other 3-aryl esters of II may be prepared by this method whereas the 3-aliphatic esters may be prepared by catalytic reduction of the corresponding ester of I. II (38 mg.) covered with 8 cc. 90% MeOH and 0.8 g. K2CO3, and refluxed 45 min. with

addition of Me2SO4 yielded the 3-Me ether of II as an oil (IV), giving with Ac2O in C5H5N 17 mg. 3-methoxy-16β-acetoxy-1,3,5-estratriene (V), m. 130-1°. To prepare 16-esters of II, a compound such as the 3-benzyl ether of II was treated with an acid chloride or anhydride and the benzyl group removed by hydrogenolysis with Pd-C. The diesters of II were prepared by using a large excess of the corresponding acid anhydride in C5H5N. The 3-Me ether of I (190 mg.) with NaBH4 in MeOH gave IV, m. 103.5-4.0°. IV with Ac2O-C5H5N yielded V, m. 132-2.5°, saponified to IV. I gave the 3-benzyl ether, reduced with NaBH4 to the 3-benzyl ether of II, m. 148-9°.

IT **1225-58-7**, 1,3,5(10)-Estratriene-3,16β-diol
(preparation of)
RN 1225-58-7 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, (16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

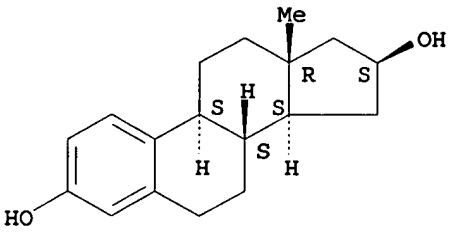


CC 10 (Organic Chemistry)
IT **1225-58-7**, 1,3,5(10)-Estratriene-3,16β-diol
1225-58-7, 3,16β-Estradiol 1229-33-0,
1,3,5(10)-Estratrien-16β-ol, 3-methoxy-
(preparation of)

L52 ANSWER 23 OF 24 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1956:8696 HCAPLUS
DOCUMENT NUMBER: 50:8696
ORIGINAL REFERENCE NO.: 50:1874e-f
TITLE: Application of the Favorskii reaction to steroid 3-ketones
AUTHOR(S): Evans, D. E.; de Paulet, A. C.; Shoppee, C. W.; Winternitz, F.
CORPORATE SOURCE: Univ. Wales
SOURCE: Chemistry & Industry (London, United Kingdom) (1955) 355-6
CODEN: CHINAG; ISSN: 0009-3068
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB cf. Bulletin society chim. France 1954, 288. 4β-Bromocoprostan-3-one with NaOMe yields Me A-norcoprostane-3-carboxylate (I), m. 67-8°, and the isomeric 2-carboxylate (II), a liquid Barbier-Wieland degradation of I yields A-norcoprostan-3-one, m. 73°. A similar degradation of II should furnish A-norcoprostan-2-one.

IT **1225-58-7**, 1,3,5(10)-Estratriene-3,16β-diol
(and esters)
RN 1225-58-7 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, (16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 10 (Organic Chemistry)
IT **1225-58-7**, 1,3,5(10)-Estratriene-3,16β-diol
(and esters)

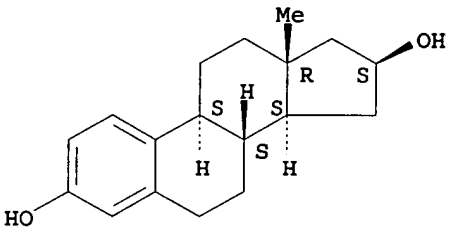
L52 ANSWER 24 OF 24 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1955:85867 HCAPLUS
DOCUMENT NUMBER: 49:85867
ORIGINAL REFERENCE NO.: 49:16212b-f
TITLE: Depression of estrone-induced uterine growth by phenolic estrogens with oxygenated functions at positions 6 or 16: the impeded estrogens
AUTHOR(S): Huggins, Charles; Jensen, Elwood V.
CORPORATE SOURCE: Univ. of Chicago
SOURCE: Journal of Experimental Medicine (1955), 102, 335-46
CODEN: JEMEAV; ISSN: 0022-1007
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB Thirty-eight-day-old, hypophysectomized rats, maintained on a ration free of growth-promoting steroids, were injected subcutaneously for 7 days with estrogenic substances (I). At necropsy, the spleen, preputial glands, vagina, and the uterus were excised and weighed, the N content of the uterus was determined, and the vaginal epithelium was examined microscopically. The growth of the uterus was related to the dosage of I which differed in the number of substituent groups and in their state of oxidation. A small increase of I dosage above the threshold amount resulted in a sharp increase of uterine growth succeeded by a gentle terrace-like rise until maximum growth was attained. The following I, termed unimpeded I, together with their terrace-point dosage, stimulated growth of the uterus: 17β-estradiol, 0.025 γ; estrone, 0.25; equilin, 0.25; 6-dehydroestrone, 2.5; D-equilenin, 5; 4-hydroxyestradiol-17β, 10; 7-ketoestrone, 10; 17α-estradiol, 10; 17-deoxyestradiol, 10; 16-estrone, 10; Δ-16,17-deoxyestradiol, 20; 16-ketoestradiol-17β, 25; 3-deoxyestradiol-17β, 25; 3-deoxyestrone, 50; 3-deoxyestradiol-17α, 100; 16-ketoestrone, >100. The presence of 2 H atoms at C6 was required for full physiol. activity of I. In contrast a I series having either a C:O group at position 6 or a C-OH at 16, when injected simultaneously with estrone, caused a moderate depression of uterine growth below that induced by estrone alone. These impeded compds. were: 6-ketoestradiol-17β, 6-ketoestrone, estriol, 16-epiestriol, 17-epiestriol, 16α-estradiol, 16β-estradiol. The optimum dosage of the compds. in the above order were 1.0 γ, 5.0, 2.5, 2.5, 5.0, and 5.0 γ, resp. The depression of uterine growth manifested itself both in a decrease in weight and in total N content. The maximum inhibition of uterine growth was 26-43%. These impeded I did not depress the growth of or the amount of cornification of the epithelial cells in the vagina. The impeded I were 3-hydroxyestratriene derivs. possessing either a C:O group at position 6 or a C-OH group at position 16.

IT **1225-58-7**, 1,3,5(10)-Estratriene-3,16β-diol

(effect on uterus)
RN 1225-58-7 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, (16β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 11H (Biological Chemistry: Pharmacology)
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(effect on uterus)

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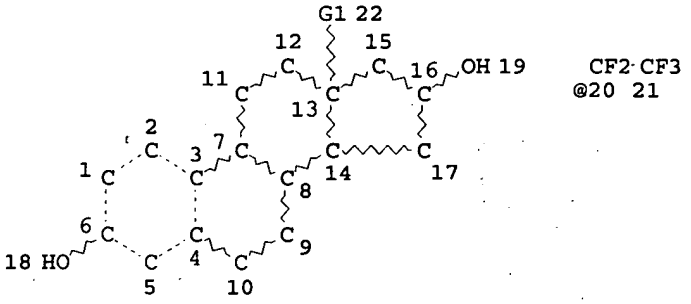

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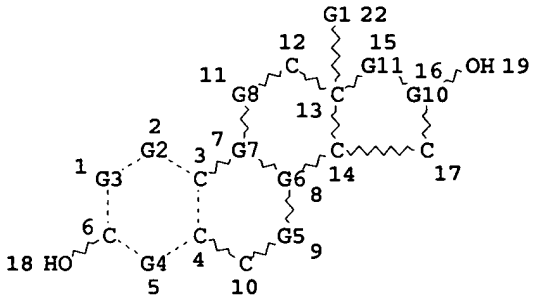

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NUMBER OF NODES IS 68

STEREO ATTRIBUTES: NONE
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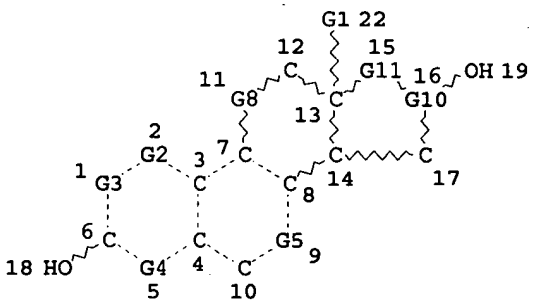

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L53  ANSWER 1 OF 16  HCAPLUS  COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER:         2005:1260644  HCAPLUS
DOCUMENT NUMBER:          144:23044
TITLE:                    Preparation of aminosulfonyl- or
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                          as estriol and estetrol prodrugs
INVENTOR(S):              Wyrwa, Ralf; Droescher, Peter; Ring, Sven;
                          Elger, Walter; Schneider, Birgitt; Hillisch,
                          Alexander; Reddersen, Gudrun
PATENT ASSIGNEE(S):       Schering Aktiengesellschaft, Germany
SOURCE:                   PCT Int. Appl., 43 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 German
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

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OTHER SOURCE(S):          CASREACT 144:23044
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* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT
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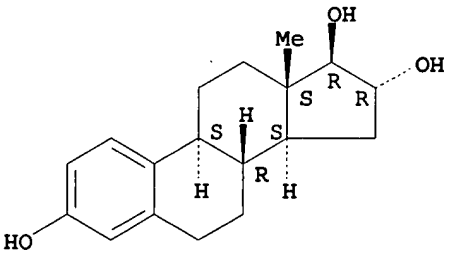
AB The invention relates to estriol and estetrol prodrugs I [A = (CH2)n; n = 0 - 4; when R1 = SO2NH2, NHSO2NH2, then R2, R3, X, X1 = H, halogen, CN, NO2, C1-5-alkyl, CpF2p+1, OC(:O)R20, CO2R20, OR20, C(:O)NHR20, OC(:O)NHR21; when R2 = SO2NH2, NHSO2NH2, then R1, R3, X, X1 = H, halogen, CN, NO2, C1-5-alkyl, CpF2p+1, OC(:O)R20, CO2R20, OR20, C(:O)NHR20, OC(:O)NHR21; when R3 = SO2NH2, NHSO2NH2, then R1, R2, X, X1 = H, halogen, CN, NO2, C1-5-alkyl, CpF2p+1, OC(:O)R20, CO2R20, OR20, C(:O)NHR20, OC(:O)NHR21; p = 1 - 3; R15 = H, OH, tri(C1-6-alkyl)silyloxy, OC(:O)R20, C2-5-heterocyclkoalkoxy; R16, R17 = OH, tri(C1-6-alkyl)silyloxy, OC(:O)R20, C2-5-heterocyclkoalkoxy; R20 = H; R20, R21, R22 = C1-5-alkyl, C3-8-cycloalkyl, aryl, (C1-4-alkylene)aryl, (C1-4-alkylene)-(C3-8-cycloalkyl), (C3-8-cycloalkylene)-(C1-4-alkyl)] , II [R4 = OH, tri(C1-6-alkyl)silyloxy, OC(:O)R20, C2-5-heterocyclkoalkoxy], III and IV, and their pharmaceutically acceptable salts, the method for production thereof, pharmaceutical compns. comprising said compds. and the use thereof for production of medicaments with **estrogenic** effect. Thus, 3,16α-dihydroxyestra-1,3,5(10)-trien-17β-yl 3'sulfamoylbenzoate [II; R4 = OH, R15 = H, R16 = α-OH, Y = (O2CC6H4SO2NH2-3)-β] was prepared from 3,16α-di[(tert-butylsilyl)oxy]estra-1,3,5(10)-trien-17β-ol via acylation with 3-(ClSO2)C6H4COCl in CHCl3 containing pyridine and amidation with aqueous NH3. The bioactivity of II [R4 = OH, R15 = H, R16 = α-OH, Y = (O2CC6H4SO2NH2-3)-β] was determined [relative binding affinity (RBA) to erythrocytes: RBA = 0.5; IC50 = 600 nM vs. carboanhydrase].

IT **50-27-1**, Estriol
RL: PAC (Pharmacological activity); RCT (Reactant); **THU (Therapeutic use)**; BIOL (Biological study); RACT (Reactant or reagent); USES (Uses)
(acylation of, by (aminosulfonylphenyl)- or (aminosulfonylaminophenyl) carboxylic acids; preparation of aminosulfonyl- or aminosulfonylamino-substituted Ph esters as estriol and estetrol prodrugs)

RN 50-27-1 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16,17-triol, (16α,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

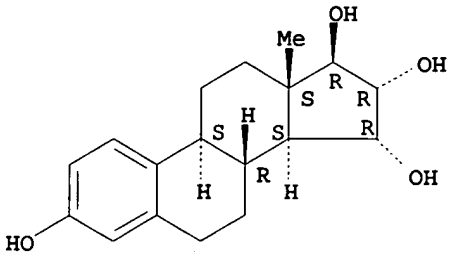


IT **15183-37-6DP**, Estetrol, prodrugs **870127-75-6P 870127-76-7P 870127-83-6P 870127-85-8P 870127-86-9P 870127-89-2P 870127-90-5P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of aminosulfonyl- or aminosulfonylamino-substituted Ph esters as estriol and estetrol prodrugs)

RN 15183-37-6 HCAPLUS

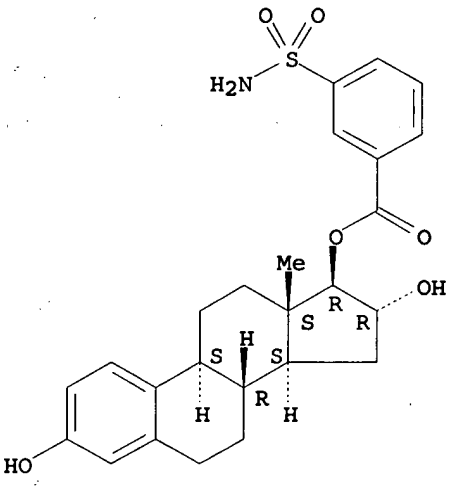
CN Estra-1,3,5(10)-triene-3,15,16,17-tetrol, (15α,16α,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



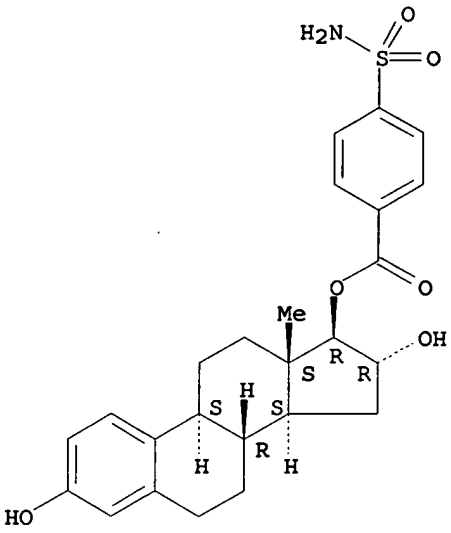
RN 870127-75-6 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16,17-triol, 17-[3-(aminosulfonyl)benzoate], (16α,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



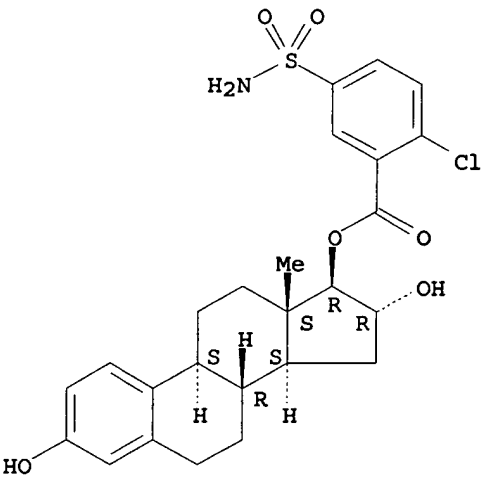
RN 870127-76-7 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16,17-triol, 17-[4-(aminosulfonyl)benzoate], (16α,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



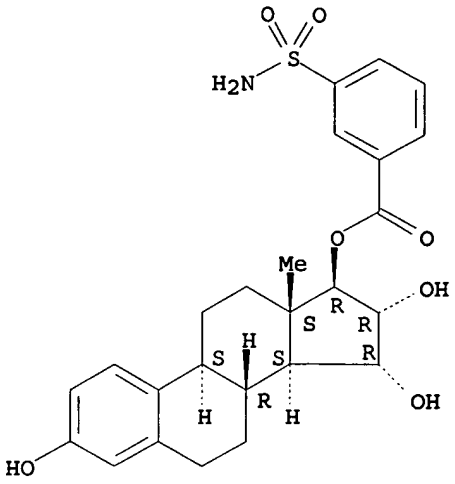
RN 870127-83-6 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16,17-triol, 17-[5-(aminosulfonyl)-2-chlorobenzoate], (16α,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



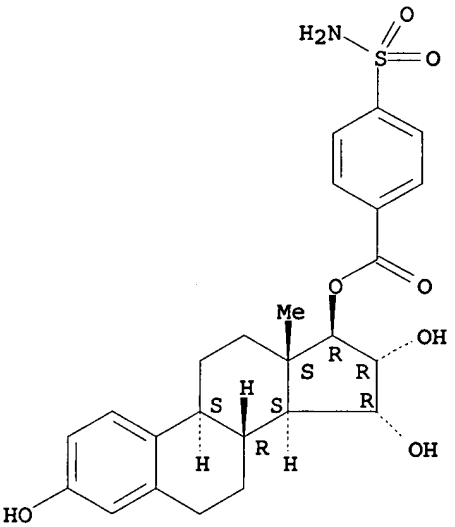
RN 870127-85-8 HCAPLUS
CN Estra-1,3,5(10)-triene-3,15,16,17-tetrol, 17-[3-(aminosulfonyl)benzoate], (15α,16α,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



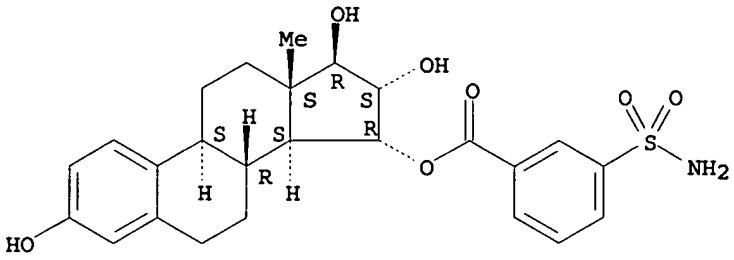
RN 870127-86-9 HCAPLUS
CN Estra-1,3,5(10)-triene-3,15,16,17-tetrol, 17-[4-(aminosulfonyl)benzoate], (15α,16α,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



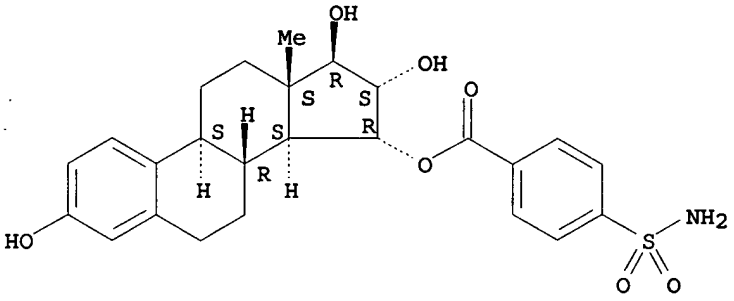
RN 870127-89-2 HCAPLUS
CN Estra-1,3,5(10)-triene-3,15,16,17-tetrol, 15-[3-(aminosulfonyl)benzoate], (15α,16α,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 870127-90-5 HCAPLUS
CN Estra-1,3,5(10)-triene-3,15,16,17-tetrol, 15-[4-(aminosulfonyl)benzoate], (15α,16α,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC ICM C07J041-00
ICS A61K031-565; A61P005-30
CC 32-3 (**Steroids**)
Section cross-reference(s): **1**, 2, 25, **63**
ST prodrug estriol estetrol aminosulfonylphenyl aminosulfonylaminophenyl ester prepn; **estrogenic** aminosulfonylphenyl aminosulfonylaminophenyl ester prodrug prepn
IT **Estrogens**
RL: RCT (Reactant); RACT (Reactant or reagent)
(acylation of, by aminosulfonylphenyl and aminosulfonylaminophenylalkanoic acids; preparation of aminosulfonyl- or aminosulfonylamino-substituted Ph esters as estriol and estetrol prodrugs)
IT Carboxylic acids, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(aminosulfonylphenyl and aminosulfonylaminophenyl, acylation by, of **estrogens**; preparation of aminosulfonyl- or aminosulfonylamino-substituted Ph esters as estriol and estetrol prodrugs)
IT Progestogens
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(combination chemotherapy of, with **estrogen** prodrugs; preparation of aminosulfonyl- or aminosulfonylamino-substituted Ph esters as estriol and estetrol prodrugs)
IT Acylation
(of **estrogens** by aminosulfonylaminophenyl- and aminosulfonylphenylalkanoic acids; preparation of aminosulfonyl- or aminosulfonylamino-substituted Ph esters as estriol and estetrol prodrugs)
IT Combination chemotherapy
(of gestagens with **estrogen** prodrugs; preparation of

aminosulfonyl- or aminosulfonylamino-substituted Ph esters as estriol and estetrol prodrugs)

IT **Estrogen** receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(α, relative binding affinity; preparation of aminosulfonyl- or aminosulfonylamino-substituted Ph esters as estriol and estetrol prodrugs)

IT **Estrogen** receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(β, relative binding affinity; preparation of aminosulfonyl- or aminosulfonylamino-substituted Ph esters as estriol and estetrol prodrugs)

IT **50-27-1**, Estriol
RL: PAC (Pharmacological activity); RCT (Reactant); **THU (Therapeutic use)**; BIOL (Biological study); RACT (Reactant or reagent); USES (Uses)
(acylation of, by (aminosulfonylphenyl)- or (aminosulfonylaminophenyl) carboxylic acids; preparation of aminosulfonyl- or aminosulfonylamino-substituted Ph esters as estriol and estetrol prodrugs)

IT 57-83-0, Progesterone, biological studies
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(combination chemotherapy of, with **estrogen** prodrugs; preparation of aminosulfonyl- or aminosulfonylamino-substituted Ph esters as estriol and estetrol prodrugs)

IT 68-22-4, Norethisterone 71-58-9, Medroxyprogesterone acetate 302-22-7, Chlormadinone acetate 427-51-0, Cyproterone acetate 797-63-7, Levonorgestrel 60282-87-3, Gestodene 65928-58-7, Dienogest 67392-87-4, Drospirenone
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(combination chemotherapy of, with **estrogen** prodrugs; preparation of aminosulfonyl- or aminosulfonylamino-substituted Ph esters as estriol and estetrol prodrugs)

IT **15183-37-6DP**, Estetrol, prodrugs **870127-75-6P** **870127-76-7P** 870127-77-8P 870127-78-9P 870127-79-0P 870127-80-3P 870127-81-4P 870127-82-5P **870127-83-6P** 870127-84-7P **870127-85-8P** **870127-86-9P** 870127-87-0P 870127-88-1P **870127-89-2P** **870127-90-5P** 870127-91-6P 870127-92-7P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of aminosulfonyl- or aminosulfonylamino-substituted Ph esters as estriol and estetrol prodrugs)

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L53 ANSWER 2 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:902909 HCAPLUS
DOCUMENT NUMBER: 143:230061
TITLE: Preparation of 7α-substituted 17-alkylene-16α-hydroxysteroidal **estrogens** for cancer treatment
INVENTOR(S): Pettersson, Lars
PATENT ASSIGNEE(S): Innoventus Project AB, Swed.
SOURCE: PCT Int. Appl., 80 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

WO 2005077968 A2 20050825 WO 2005-SE188
2005
0211
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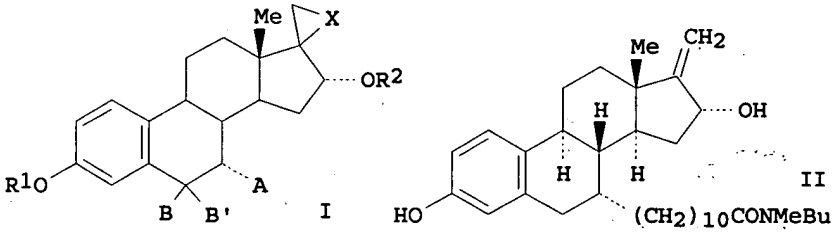


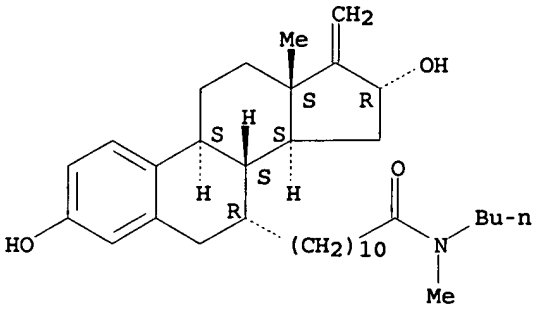
AB 7α-Substituted 17-alkylene-16α-hydroxysteroidal **estrogens** of formula I [A = 8-22 atom substituent; B, B' = H, OH, alkoxy, etc.; X = methylene, bond; R1 = H, metabolically unstable group; R2 = H, acyl, benzoyl] are prepared which exhibit anti-**estrogenic** properties. The present invention also relates to use of said compds. as a medicament, and for the treatment of **estrogen** dependent disorders, a pharmaceutical composition comprising one or more of said compds. and a method of treatment. Thus, II was prepared, and showed 61% antagonism in vivo in immature female mice.

IT **862700-33-2P 862700-40-1P 862700-44-5P**
862700-47-8P 862700-49-0P 862700-51-4P
862700-53-6P 862700-55-8P 862700-57-0P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of antiestrogenic 17-alkylene-16α-hydroxyestratrienes for cancer treatment)

RN 862700-33-2 HCAPLUS

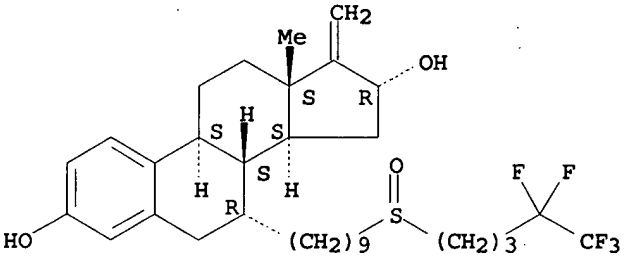
CN Estra-1,3,5(10)-triene-7-undecanamide, N-butyl-3,16-dihydroxy-N-methyl-17-methylene-, (7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



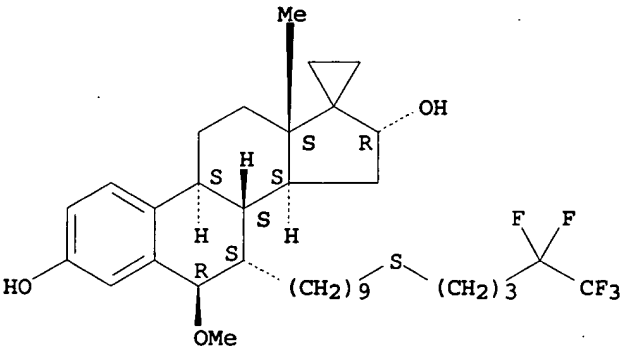
RN 862700-40-1 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 17-methylene-7-[9-[(4,4,5,5,5-pentafluoropentyl)sulfinyl]nonyl]-, (7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



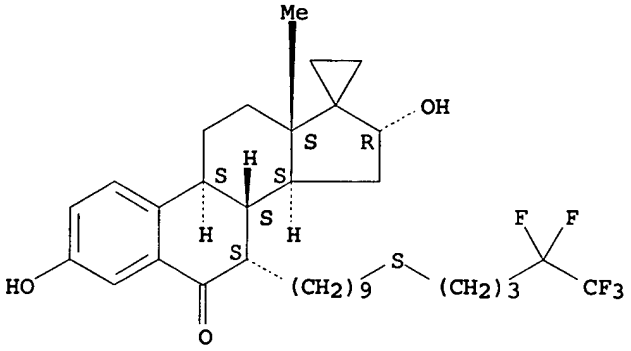
RN 862700-44-5 HCAPLUS
CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-3,16-diol, 6-methoxy-7-[9-[(4,4,5,5,5-pentafluoropentyl)thio]nonyl]-, (6β,7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



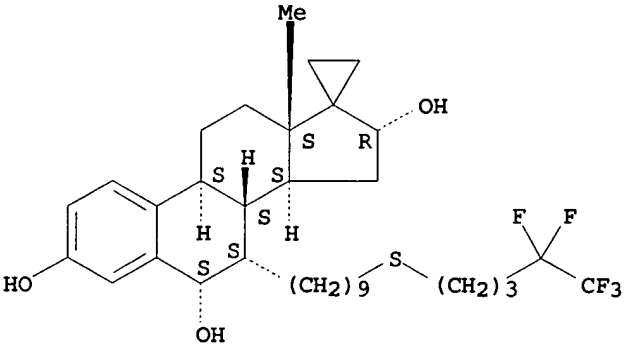
RN 862700-47-8 HCAPLUS
CN 17,21-Cyclo-19-norpregna-1,3,5(10)-trien-6-one, 3,16-dihydroxy-7-[9-[(4,4,5,5,5-pentafluoropentyl)thio]nonyl]-, (7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



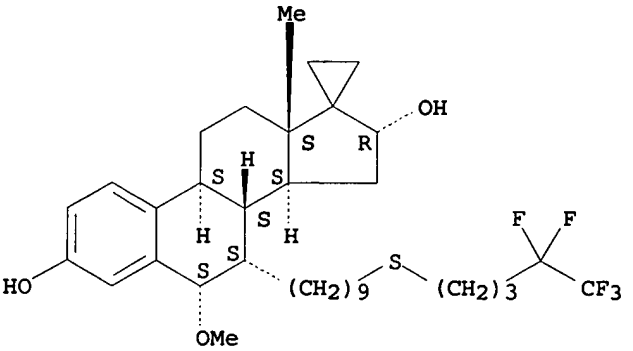
RN 862700-49-0 HCAPLUS
CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-3,6,16-triol, 7-[9-[(4,4,5,5,5-pentafluoropentyl)thio]nonyl]-, (6α,7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 862700-51-4 HCAPLUS
CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-3,16-diol, 6-methoxy-7-[9-[(4,4,5,5,5-pentafluoropentyl)thio]nonyl]-, (6α,7α,16α)- (9CI) (CA INDEX NAME)

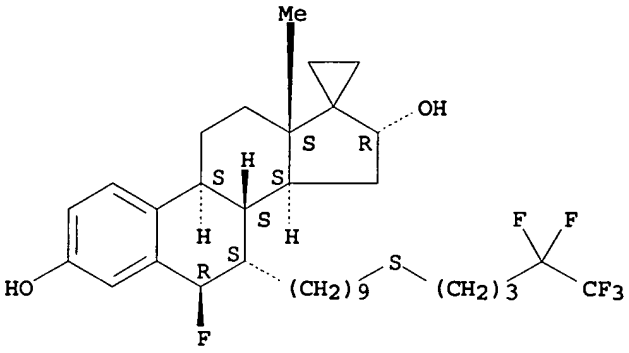
Absolute stereochemistry.



RN 862700-53-6 HCAPLUS
CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-3,16-diol,

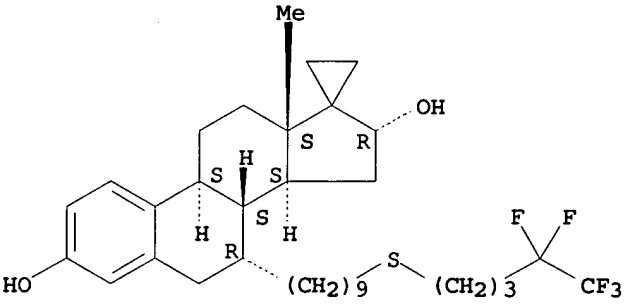
6-fluoro-7-[9-[(4,4,5,5,5-pentafluoropentyl)thio]nonyl]-,
(6β,7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



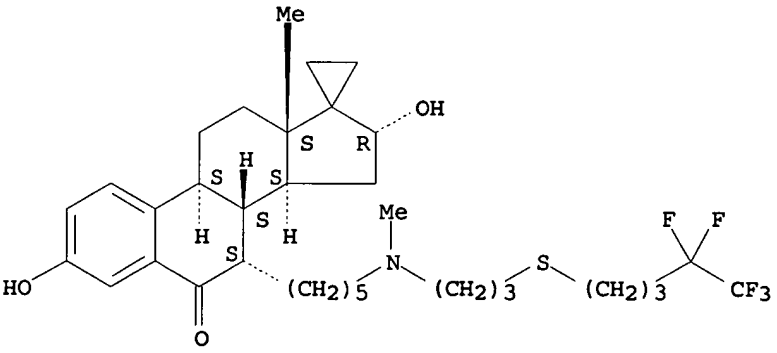
RN 862700-55-8 HCAPLUS
CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-3,16-diol,
7-[9-[(4,4,5,5,5-pentafluoropentyl)thio]nonyl]-,
(7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 862700-57-0 HCAPLUS
CN 17,21-Cyclo-19-norpregna-1,3,5(10)-trien-6-one,
3,16-dihydroxy-7-[5-[methyl[3-[(4,4,5,5,5-
pentafluoropentyl)thio]propyl]amino]pentyl]-, (7α,16α)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



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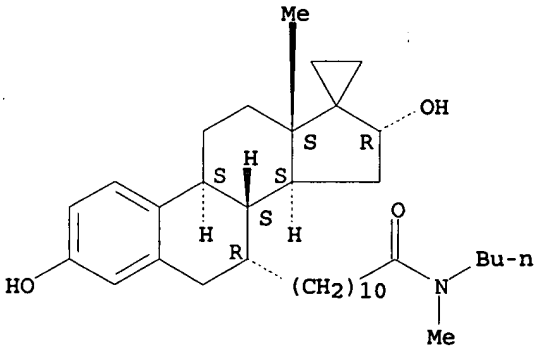
862702-41-8P 862702-42-9P 862702-43-0P
862702-44-1P 862702-45-2P 862702-47-4P
862702-48-5P 862702-50-9P 862702-51-0P
862702-52-1P 862702-53-2P 862702-54-3P
862702-55-4P 862702-56-5P 862702-57-6P
862702-59-8P 862702-60-1P 862702-61-2P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of antiestrogenic 17-alkylene-16α-hydroxyestratrienes for cancer treatment)

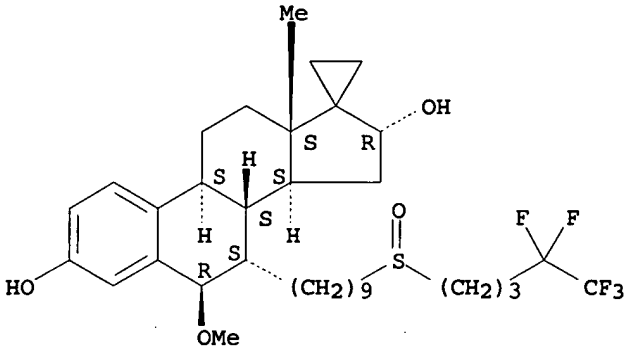
RN 862700-38-7 HCAPLUS
CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-7-undecanamide, N-butyl-3,16-dihydroxy-N-methyl-, (7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



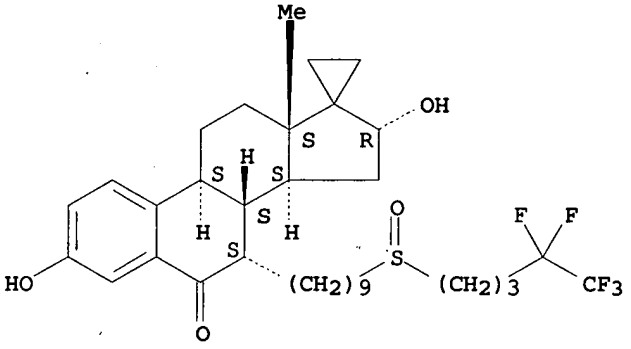
RN 862700-46-7 HCAPLUS
CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-3,16-diol, 6-methoxy-7-[9-[(4,4,5,5,5-pentafluoropentyl)sulfinyl]nonyl]-, (6β,7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



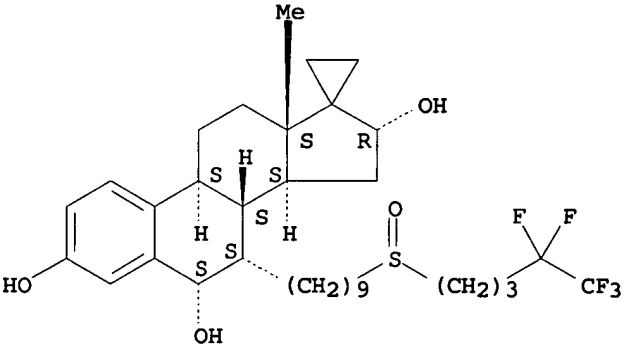
RN 862700-48-9 HCAPLUS
CN 17,21-Cyclo-19-norpregna-1,3,5(10)-trien-6-one,
3,16-dihydroxy-7-[9-[(4,4,5,5,5-pentafluoropentyl)sulfinyl]nonyl]-
, (7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 862700-50-3 HCAPLUS
CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-3,6,16-triol,
7-[9-[(4,4,5,5,5-pentafluoropentyl)sulfinyl]nonyl]-,
(6α,7α,16α)- (9CI) (CA INDEX NAME)

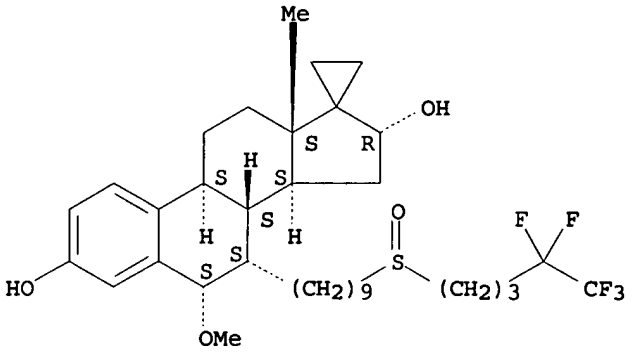
Absolute stereochemistry.



RN 862700-52-5 HCAPLUS
CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-3,16-diol,
6-methoxy-7-[9-[(4,4,5,5,5-pentafluoropentyl)sulfinyl]nonyl]-,

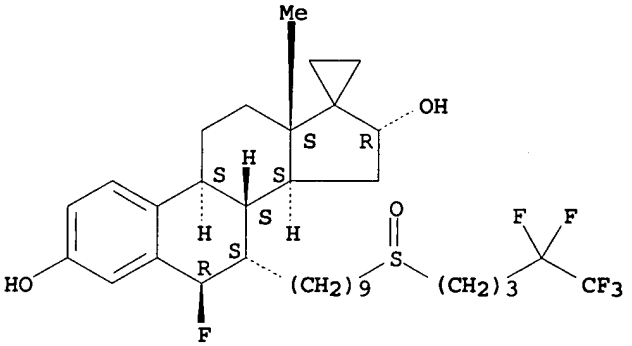
(6α,7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



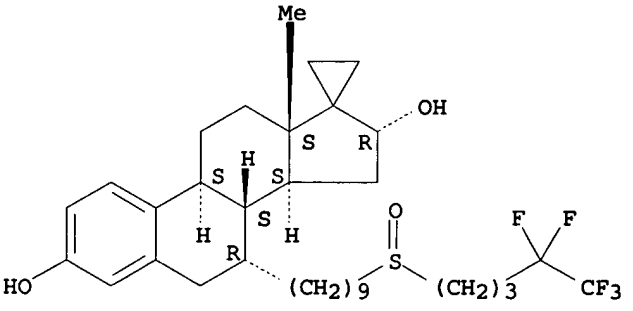
RN 862700-54-7 HCAPLUS
CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-3,16-diol,
6-fluoro-7-[9-[(4,4,5,5,5-pentafluoropentyl)sulfinyl]nonyl]-,
(6β,7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 862700-56-9 HCAPLUS
CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-3,16-diol,
7-[9-[(4,4,5,5,5-pentafluoropentyl)sulfinyl]nonyl]-,
(7α,16α)- (9CI) (CA INDEX NAME)

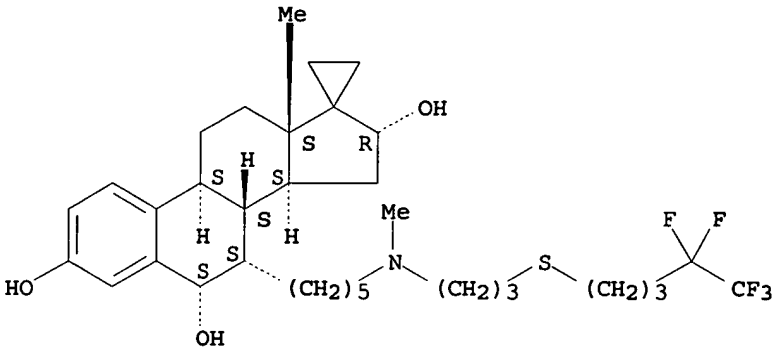
Absolute stereochemistry.



RN 862700-59-2 HCAPLUS
CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-3,6,16-triol,

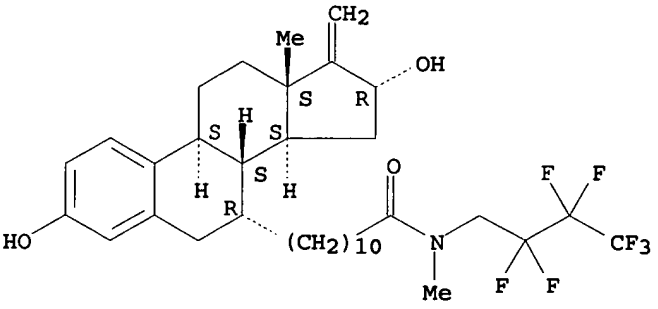
7-[5-[methyl[3-[(4,4,5,5,5-pentafluoropentyl)thio]propyl]amino]pen
tyl]-, (6α,7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



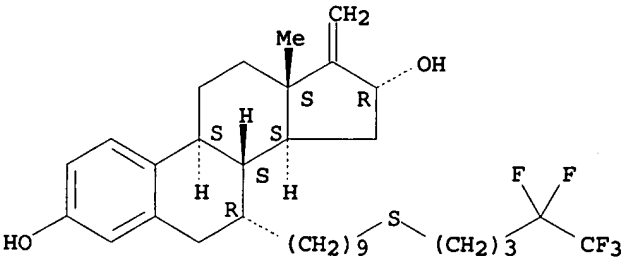
RN 862701-26-6 HCAPLUS
CN Estra-1,3,5(10)-triene-7-undecanamide, N-(2,2,3,3,4,4,4-heptafluorobutyl)-3,16-dihydroxy-N-methyl-17-methylene-, (7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



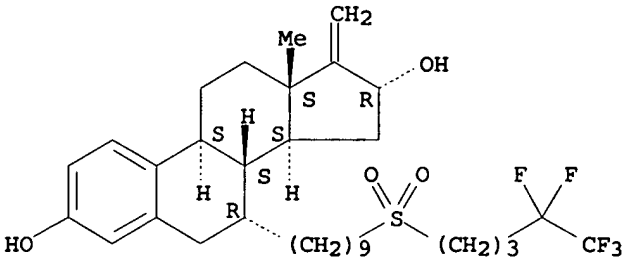
RN 862701-28-8 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 17-methylene-7-[9-[(4,4,5,5,5-pentafluoropentyl)thio]nonyl]-, (7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



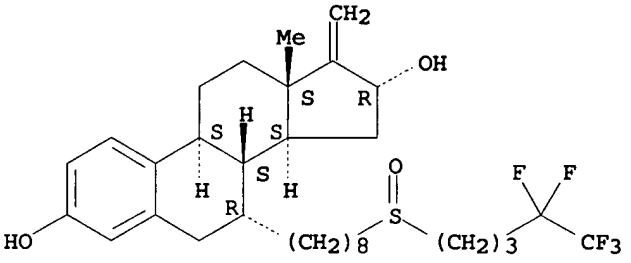
RN 862701-34-6 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 17-methylene-7-[9-[(4,4,5,5,5-pentafluoropentyl)sulfonyl]nonyl]-, (7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



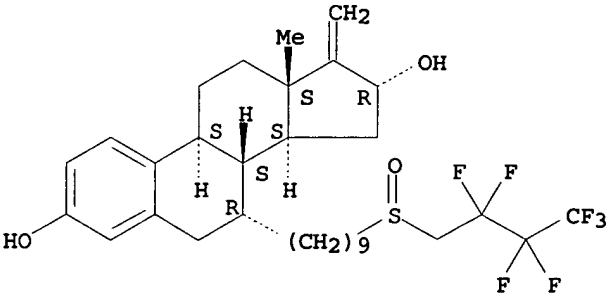
RN 862701-36-8 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 17-methylene-7-[8-[(4,4,5,5,5-pentafluoropentyl)sulfinyl]octyl]-, (7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



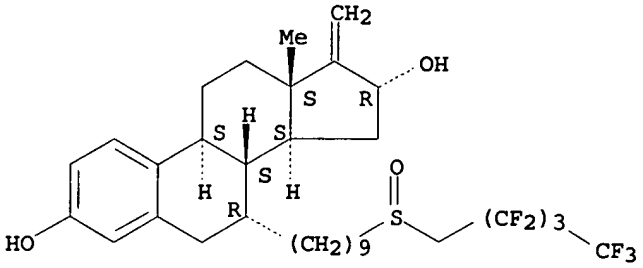
RN 862701-38-0 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 7-[9-[(2,2,3,3,4,4,4-heptafluorobutyl)sulfinyl]nonyl]-17-methylene-, (7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



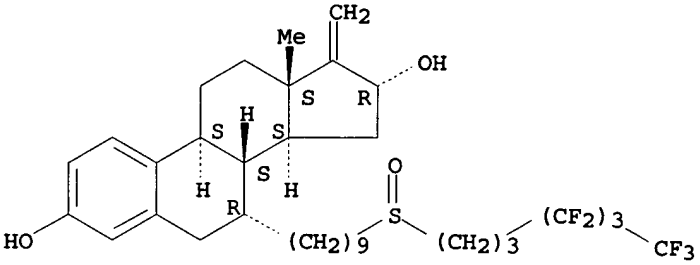
RN 862701-40-4 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 17-methylene-7-[9-[(2,2,3,3,4,4,5,5,5-nonafluoropentyl)sulfinyl]nonyl]-, (7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



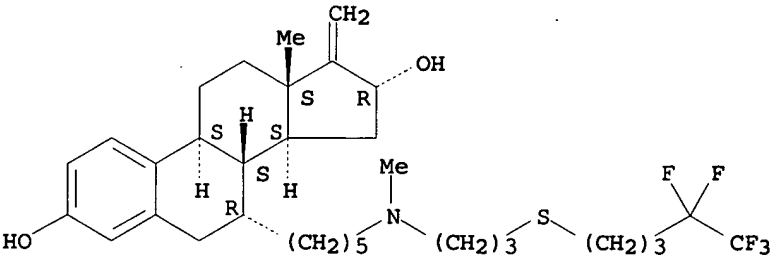
RN 862701-42-6 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 17-methylene-7-[9-[(4,4,5,5,6,6,7,7,7-nonafluoroheptyl)sulfinyl]nonyl]-, (7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



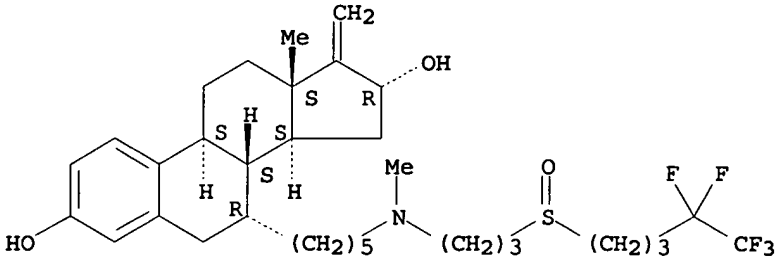
RN 862701-44-8 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 17-methylene-7-[5-[methyl[3-[(4,4,5,5,5-pentafluoropentyl)thio]propyl]amino]pentyl]-, (7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



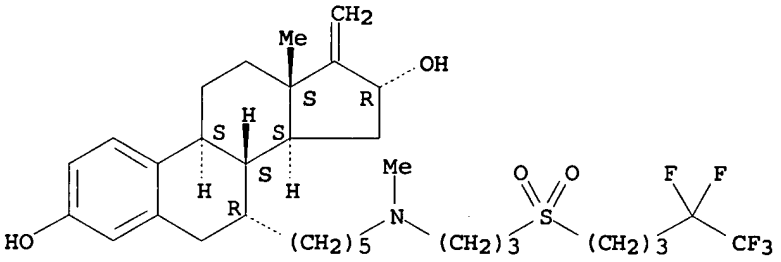
RN 862701-46-0 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 17-methylene-7-[5-[methyl[3-[(4,4,5,5,5-pentafluoropentyl)sulfinyl]propyl]amino]pentyl]-, (7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



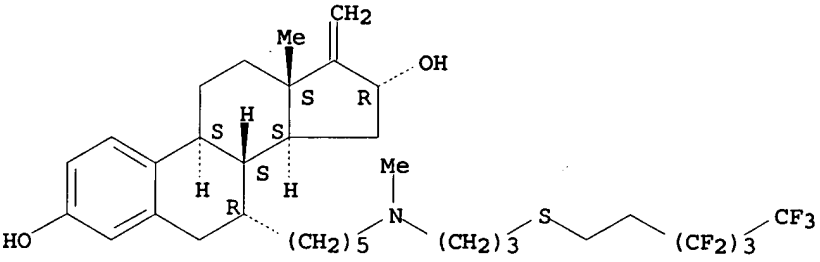
RN 862701-52-8 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 17-methylene-7-[5-[methyl[3-[(4,4,5,5,5-pentafluoropentyl)sulfonyl]propyl]amino]pentyl]-, (7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



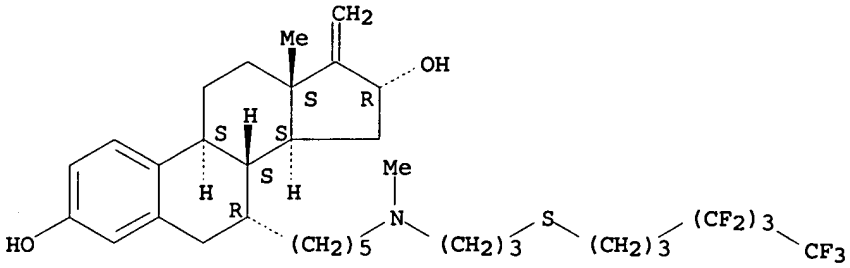
RN 862701-54-0 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 17-methylene-7-[5-[methyl[3-[(3,3,4,4,5,5,6,6,6-nonafluorohexyl)thio]propyl]amino]pentyl]-, (7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



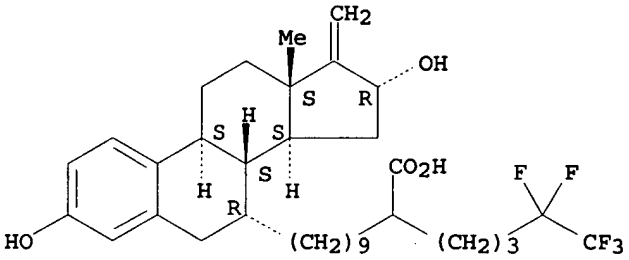
RN 862701-56-2 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 17-methylene-7-[5-[methyl[3-[(4,4,5,5,6,6,7,7,7-nonafluoroheptyl)thio]propyl]amino]pentyl]-, (7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



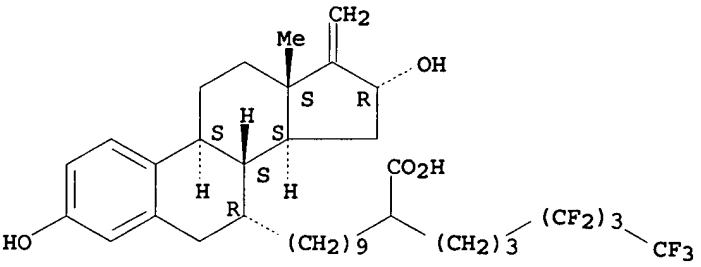
RN 862701-58-4 HCAPLUS
CN Estra-1,3,5(10)-triene-7-undecanoic acid, 3,16-dihydroxy-17-methylene-α-(4,4,5,5,5-pentafluoropentyl)-, (7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



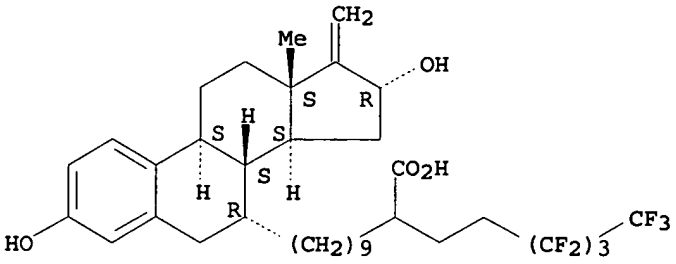
RN 862701-60-8 HCAPLUS
CN Estra-1,3,5(10)-triene-7-undecanoic acid, 3,16-dihydroxy-17-methylene-α-(4,4,5,5,6,6,7,7,7-nonafluoroheptyl)-, (7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



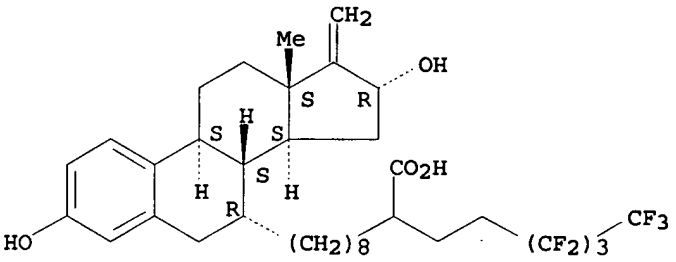
RN 862701-62-0 HCAPLUS
CN Estra-1,3,5(10)-triene-7-undecanoic acid, 3,16-dihydroxy-17-methylene-α-(3,3,4,4,5,5,6,6,6-nonafluorohexyl)-, (7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



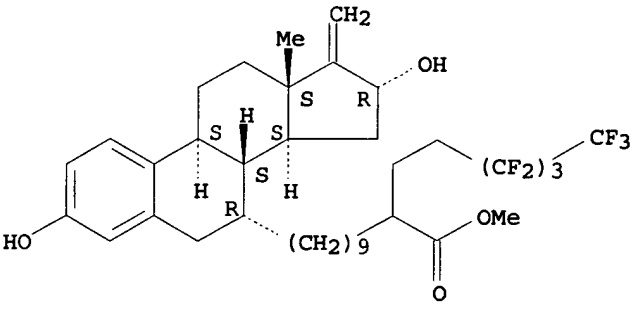
RN 862701-64-2 HCAPLUS
CN Estra-1,3,5(10)-triene-7-decanoic acid, 3,16-dihydroxy-17-methylene-α-(3,3,4,4,5,5,6,6,6-nonafluorohexyl)-, (7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



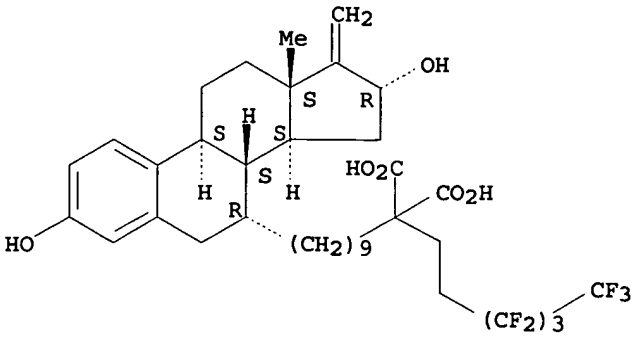
RN 862701-66-4 HCAPLUS
CN Estra-1,3,5(10)-triene-7-undecanoic acid, 3,16-dihydroxy-17-methylene-α-(3,3,4,4,5,5,6,6,6-nonafluorohexyl)-, methyl ester, (7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



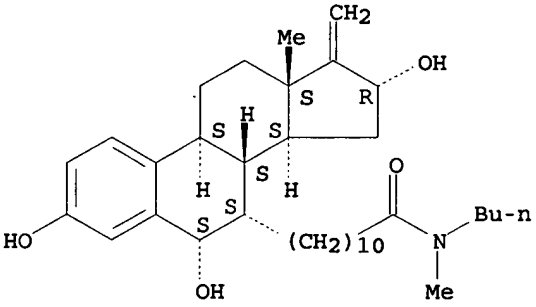
RN 862701-68-6 HCAPLUS
CN Propanedioic acid, [9-[(7α,16α)-3,16-dihydroxy-17-methyleneestra-1,3,5(10)-trien-7-yl]nonyl](3,3,4,4,5,5,6,6,6-nonafluorohexyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



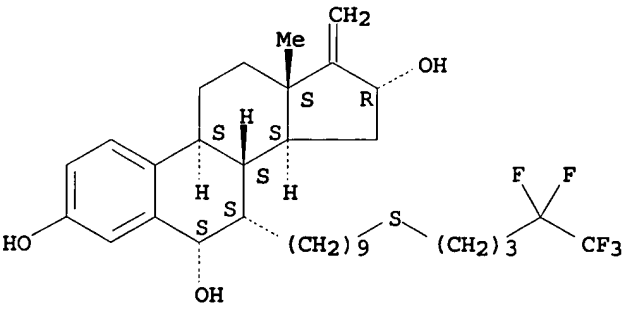
RN 862701-69-7 HCAPLUS
CN Estra-1,3,5(10)-triene-7-undecanamide, N-butyl-3,6,16-trihydroxy-N-methyl-17-methylene-, (6α,7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



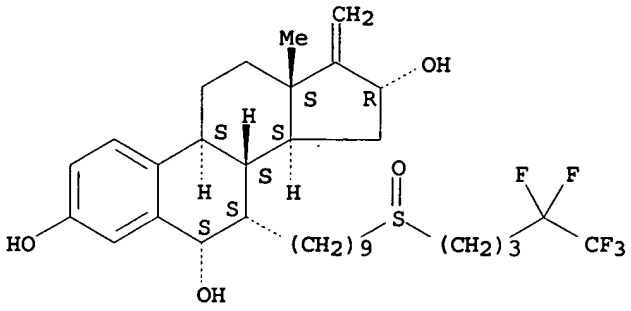
RN 862701-71-1 HCAPLUS
CN Estra-1,3,5(10)-triene-3,6,16-triol, 17-methylene-7-[9-[(4,4,5,5,5-pentafluoropentyl)thio]nonyl]-, (6α,7α,16α)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



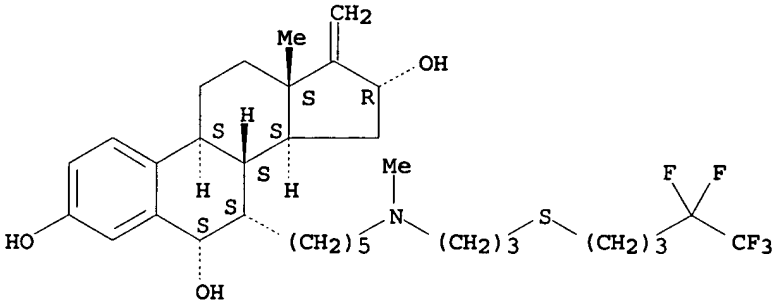
RN 862701-73-3 HCAPLUS
CN Estra-1,3,5(10)-triene-3,6,16-triol, 17-methylene-7-[9-[(4,4,5,5,5-pentafluoropentyl)sulfinyl]nonyl]-, (6α,7α,16α)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



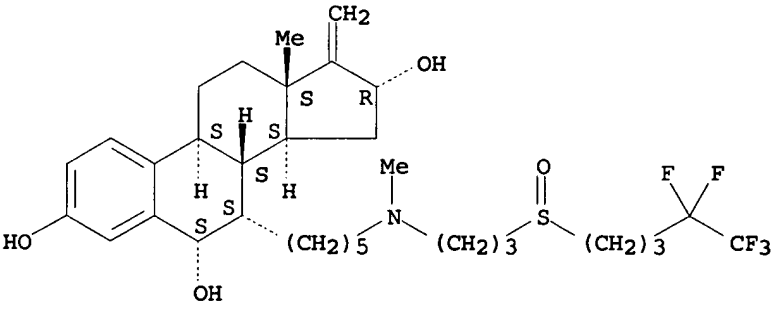
RN 862701-77-7 HCAPLUS
CN Estra-1,3,5(10)-triene-3,6,16-triol, 17-methylene-7-[5-[methyl[3-[(4,4,5,5,5-pentafluoropentyl)thio]propyl]amino]pentyl]-, (6α,7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



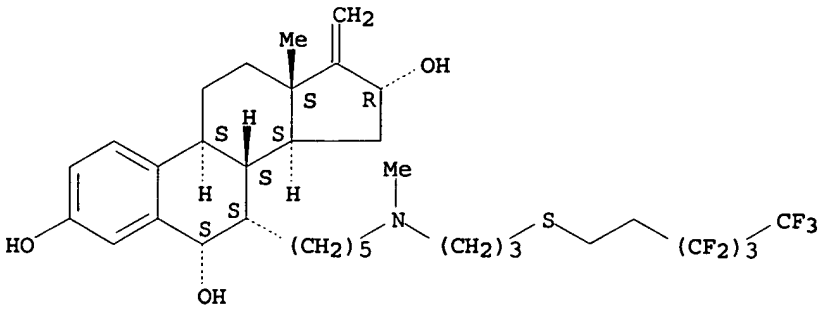
RN 862701-81-3 HCAPLUS
CN Estra-1,3,5(10)-triene-3,6,16-triol, 17-methylene-7-[5-[methyl[3-[(4,4,5,5,5-pentafluoropentyl)sulfinyl]propyl]amino]pentyl]-, (6α,7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



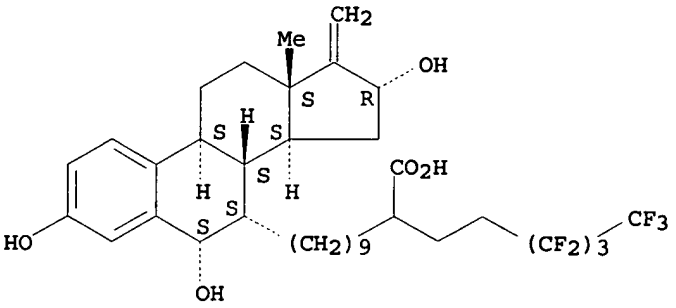
RN 862701-83-5 HCAPLUS
CN Estra-1,3,5(10)-triene-3,6,16-triol, 17-methylene-7-[5-[methyl[3-[(3,3,4,4,5,5,6,6,6-nonafluorohexyl)thio]propyl]amino]pentyl]-, (6α,7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



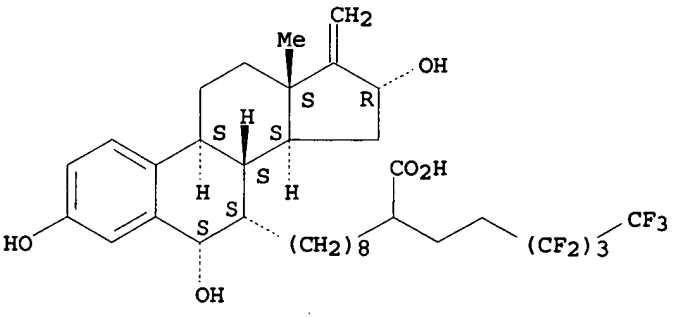
RN 862701-85-7 HCAPLUS
CN Estra-1,3,5(10)-triene-7-undecanoic acid, 3,6,16-trihydroxy-17-methylene-α-(3,3,4,4,5,5,6,6,6-nonafluorohexyl)-, (6α,7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



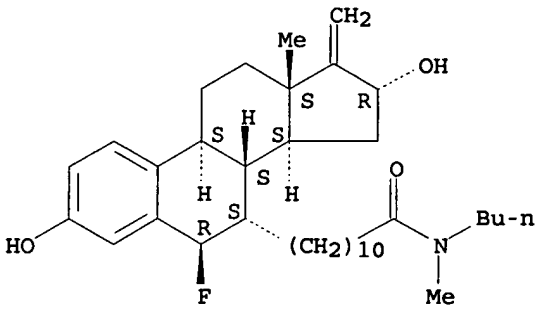
RN 862701-87-9 HCAPLUS
CN Estra-1,3,5(10)-triene-7-decanoic acid, 3,6,16-trihydroxy-17-methylene-α-(3,3,4,4,5,5,6,6,6-nonafluorohexyl)-, (6α,7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



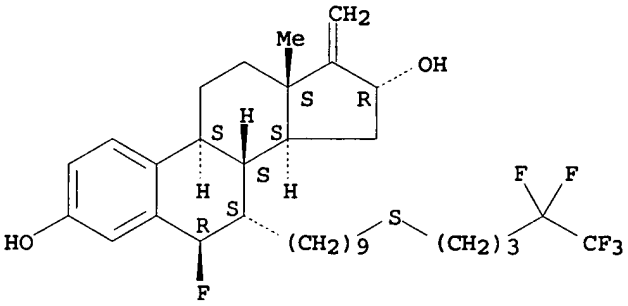
RN 862701-89-1 HCAPLUS
CN Estra-1,3,5(10)-triene-7-undecanamide, N-butyl-6-fluoro-3,16-dihydroxy-N-methyl-17-methylene-, (6β,7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



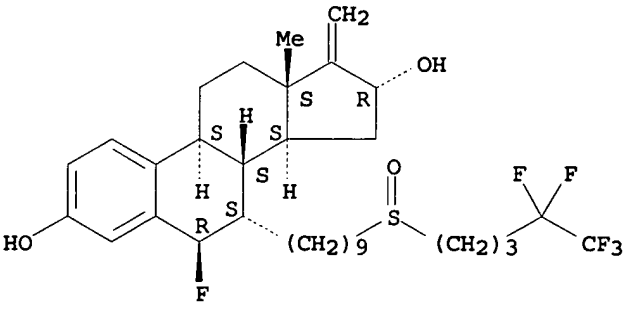
RN 862701-91-5 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 6-fluoro-17-methylene-7-[9-[(4,4,5,5,5-pentafluoropentyl)thio]nonyl]-, (6β,7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



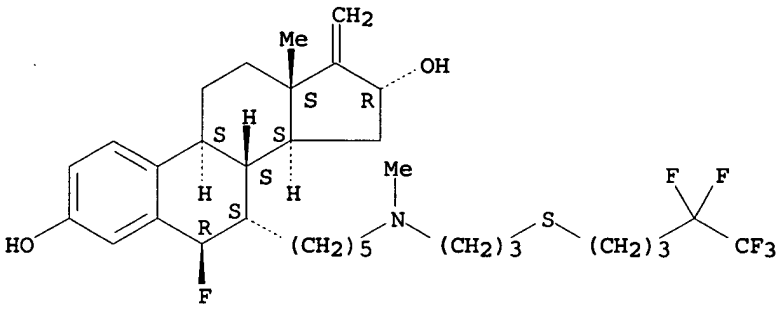
RN 862701-93-7 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 6-fluoro-17-methylene-7-[9-[(4,4,5,5,5-pentafluoropentyl)sulfinyl]nonyl]-, (6β,7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



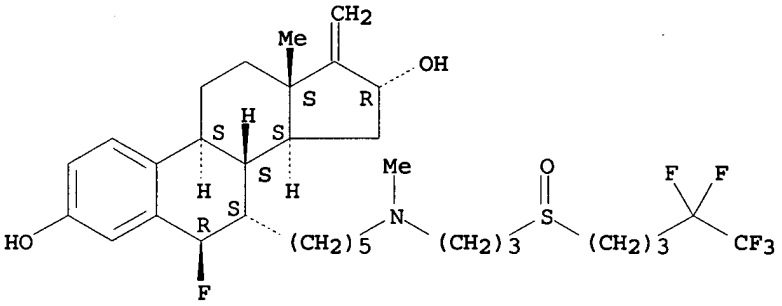
RN 862701-95-9 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 6-fluoro-17-methylene-7-[5-[methyl[3-[(4,4,5,5,5-pentafluoropentyl)thio]propyl]amino]pentyl]-, (6β,7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



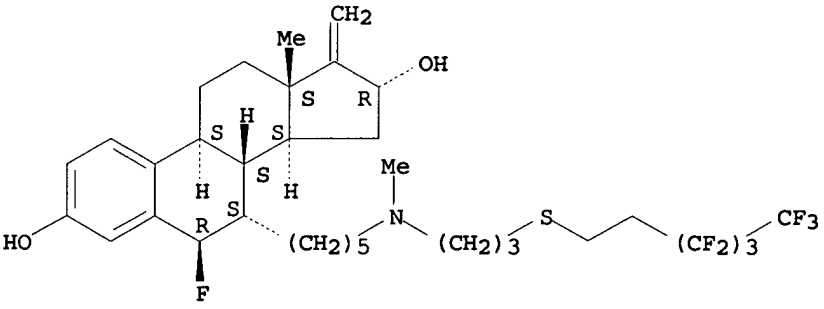
RN 862701-97-1 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 6-fluoro-17-methylene-7-[5-[methyl[3-[(4,4,5,5,5-pentafluoropentyl)sulfinyl]propyl]amino]pentyl]-, (6β,7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



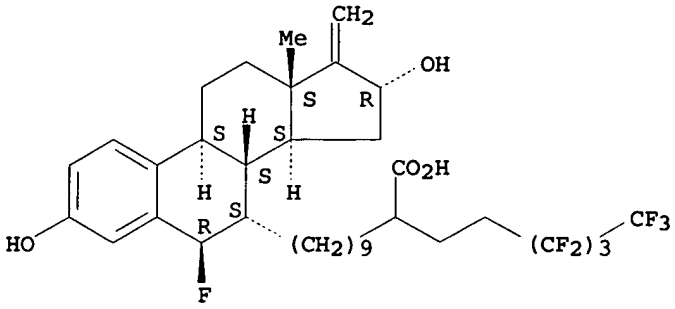
RN 862701-99-3 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 6-fluoro-17-methylene-7-[5-[methyl[3-[(3,3,4,4,5,5,6,6,6-nonafluorohexyl)thio]propyl]amino]pentyl]-, (6β,7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



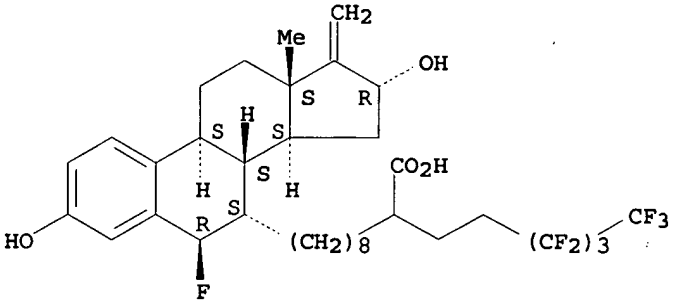
RN 862702-01-0 HCAPLUS
CN Estra-1,3,5(10)-triene-7-undecanoic acid, 6-fluoro-3,16-dihydroxy-17-methylene-α-(3,3,4,4,5,5,6,6,6-nonafluorohexyl)-, (6β,7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



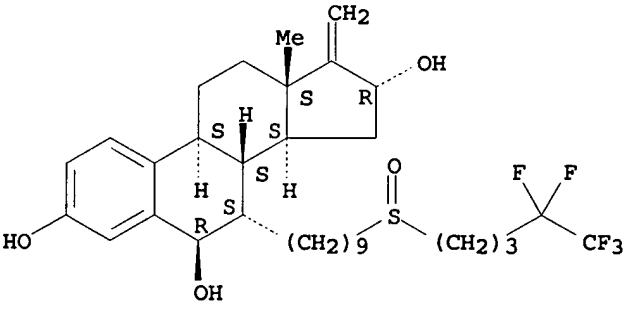
RN 862702-03-2 HCAPLUS
CN Estra-1,3,5(10)-triene-7-decanoic acid, 6-fluoro-3,16-dihydroxy-17-methylene-α-(3,3,4,4,5,5,6,6,6-nonafluorohexyl)-, (6β,7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



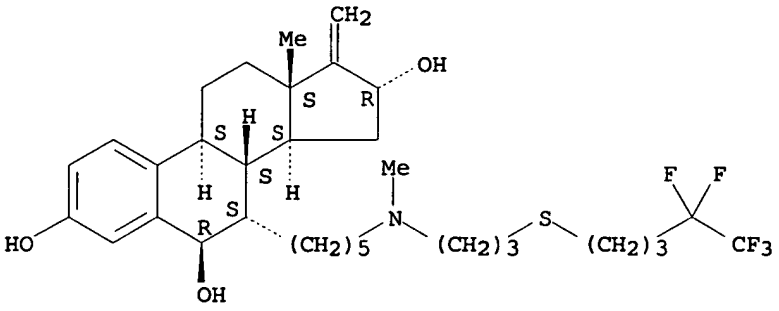
RN 862702-04-3 HCAPLUS
CN Estra-1,3,5(10)-triene-3,6,16-triol, 17-methylene-7-[9-[(4,4,5,5,5-pentafluoropentyl)sulfinyl]nonyl]-, (6β,7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



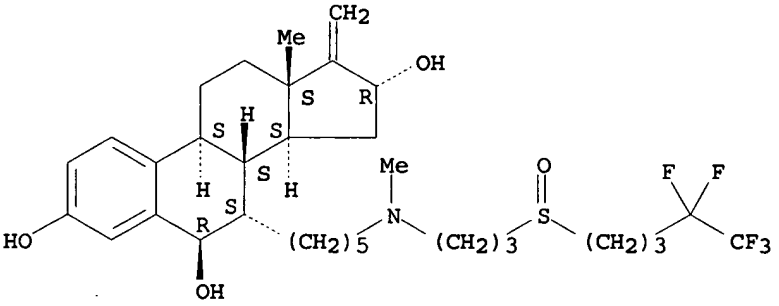
RN 862702-05-4 HCAPLUS
CN Estra-1,3,5(10)-triene-3,6,16-triol, 17-methylene-7-[5-[methyl[3-[(4,4,5,5,5-pentafluoropentyl)thio]propyl]amino]pentyl]-, (6β,7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



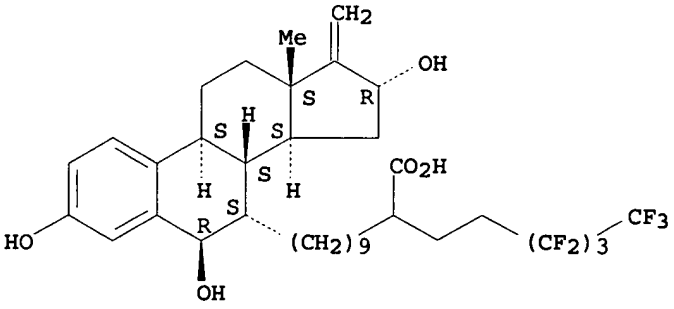
RN 862702-06-5 HCAPLUS
CN Estra-1,3,5(10)-triene-3,6,16-triol, 17-methylene-7-[5-[methyl[3-[(4,4,5,5,5-pentafluoropentyl)sulfinyl]propyl]amino]pentyl]-, (6β,7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



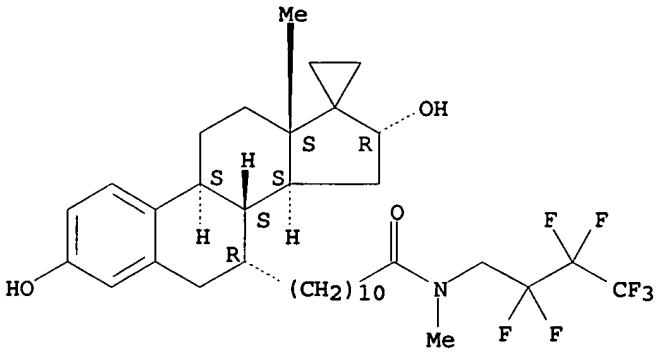
RN 862702-07-6 HCAPLUS
CN Estra-1,3,5(10)-triene-7-undecanoic acid, 3,6,16-trihydroxy-17-methylene-α-(3,3,4,4,5,5,6,6,6-nonafluorohexyl)-, (6β,7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



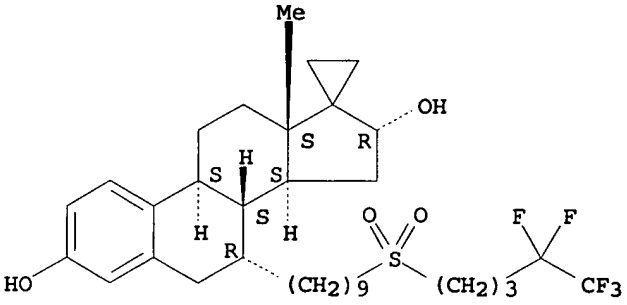
RN 862702-08-7 HCAPLUS
CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-7-undecanamide, N-(2,2,3,3,4,4,4-heptafluorobutyl)-3,16-dihydroxy-N-methyl-, (7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



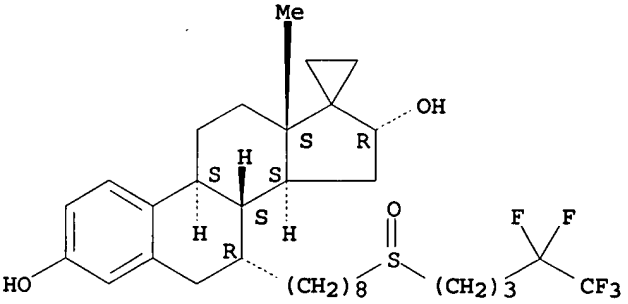
RN 862702-11-2 HCAPLUS
CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-3,16-diol, 7-[9-[(4,4,5,5,5-pentafluoropentyl)sulfonyl]nonyl]-, (7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



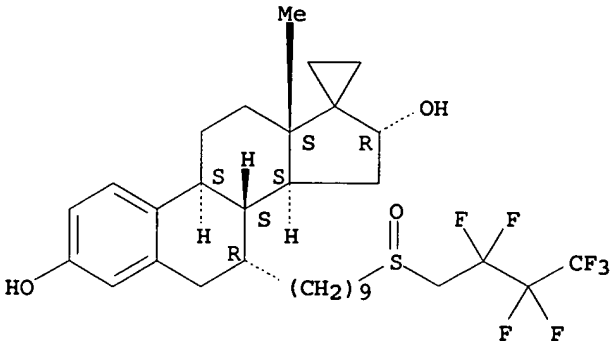
RN 862702-12-3 HCAPLUS
CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-3,16-diol, 7-[8-[(4,4,5,5,5-pentafluoropentyl)sulfinyl]octyl]-, (7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



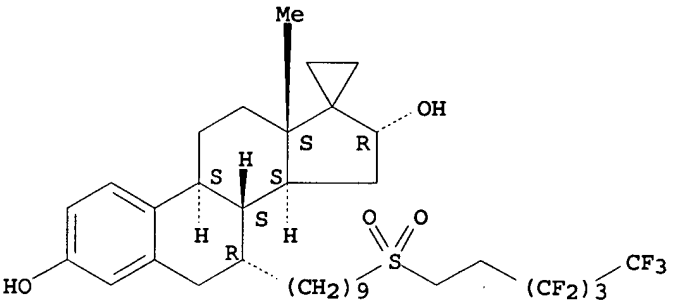
RN 862702-13-4 HCAPLUS
CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-3,16-diol, 7-[9-[(2,2,3,3,4,4,4-heptafluorobutyl)sulfinyl]nonyl]-, (7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



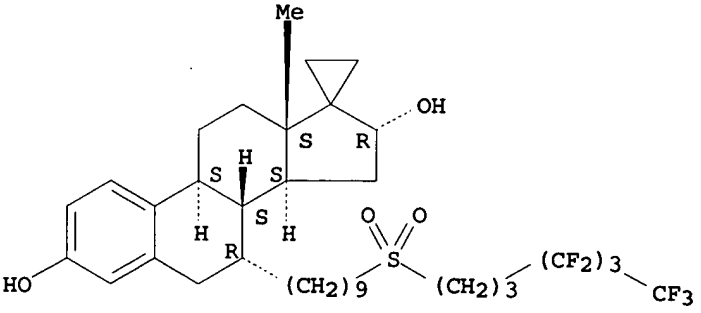
RN 862702-14-5 HCAPLUS
CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-3,16-diol, 7-[9-[(3,3,4,4,5,5,6,6,6-nonafluorohexyl)sulfonyl]nonyl]-, (7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



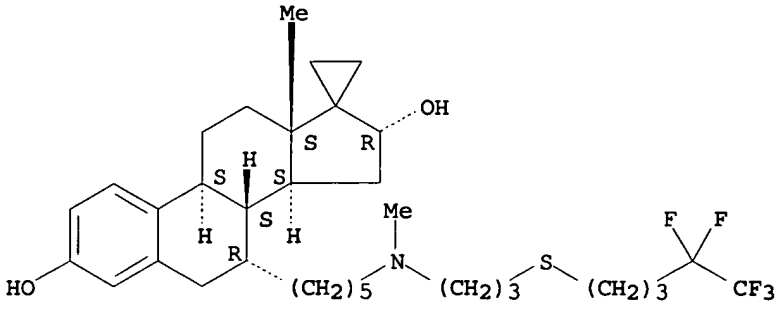
RN 862702-15-6 HCAPLUS
CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-3,16-diol, 7-[9-[(4,4,5,5,6,6,7,7,7-nonafluoroheptyl)sulfonyl]nonyl]-, (7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



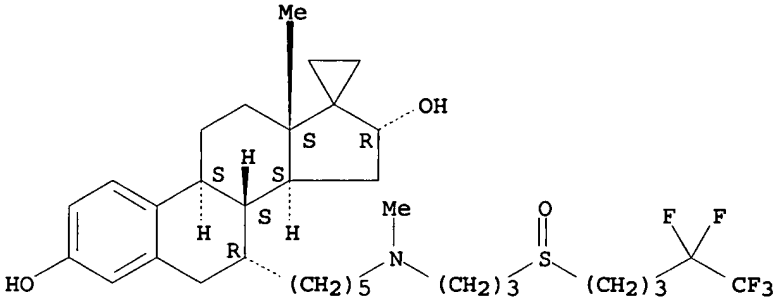
RN 862702-16-7 HCAPLUS
CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-3,16-diol, 7-[5-[methyl[3-[(4,4,5,5,5-pentafluoropentyl)thio]propyl]amino]pentyl]-, (7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



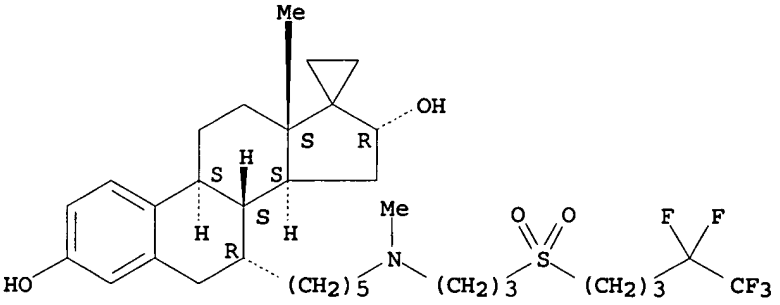
RN 862702-20-3 HCAPLUS
CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-3,16-diol, 7-[5-[methyl[3-[(4,4,5,5,5-pentafluoropentyl)sulfinyl]propyl]amino]pentyl]-, (7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



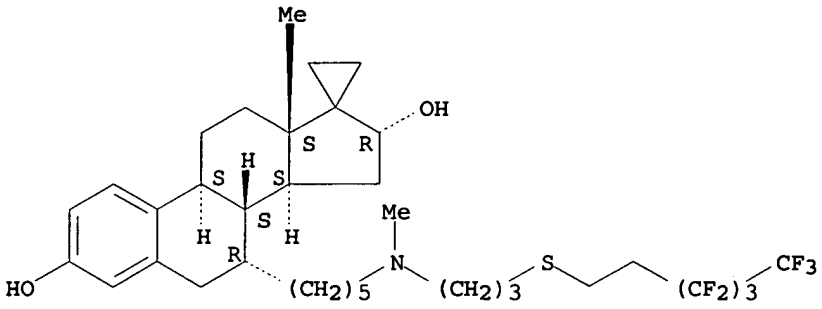
RN 862702-21-4 HCAPLUS
CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-3,16-diol, 7-[5-[methyl[3-[(4,4,5,5,5-pentafluoropentyl)sulfonyl]propyl]amino]pentyl]-, (7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



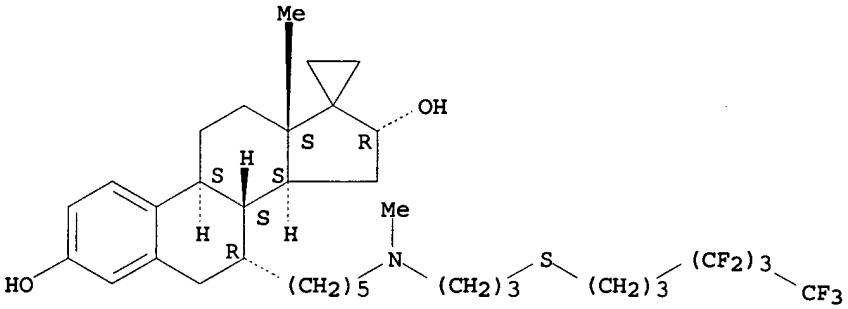
RN 862702-22-5 HCAPLUS
CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-3,16-diol, 7-[5-[methyl[3-[(3,3,4,4,5,5,6,6,6-nonafluorohexyl)thio]propyl]ami no]pentyl]-, (7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



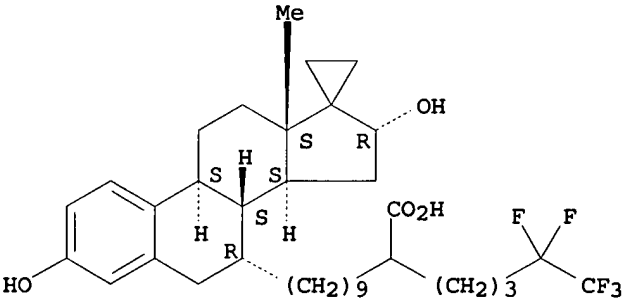
RN 862702-23-6 HCAPLUS
CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-3,16-diol, 7-[5-[methyl[3-[(4,4,5,5,6,6,7,7,7-nonafluoroheptyl)thio]propyl]amino]pentyl]-, (7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



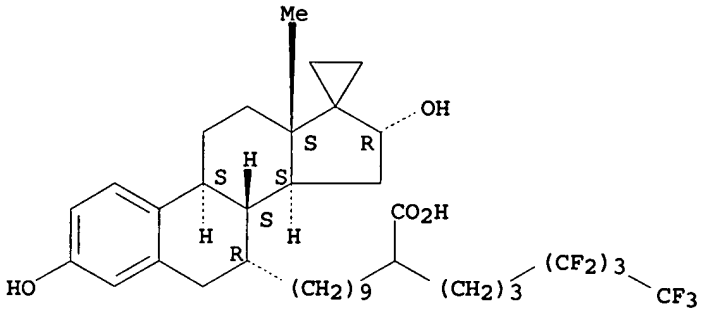
RN 862702-24-7 HCAPLUS
CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-7-undecanoic acid, 3,16-dihydroxy-α-(4,4,5,5,5-pentafluoropentyl)-, (7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



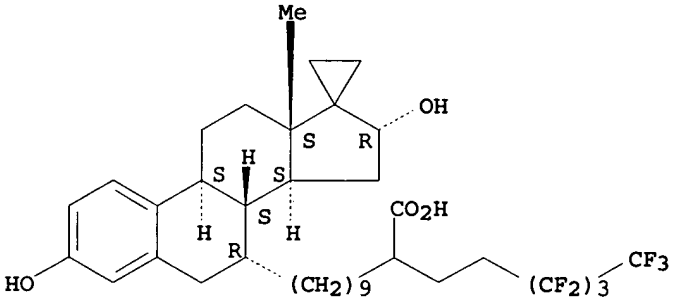
RN 862702-25-8 HCAPLUS
CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-7-undecanoic acid, 3,16-dihydroxy-α-(4,4,5,5,6,6,7,7,7-nonafluoroheptyl)-, (7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



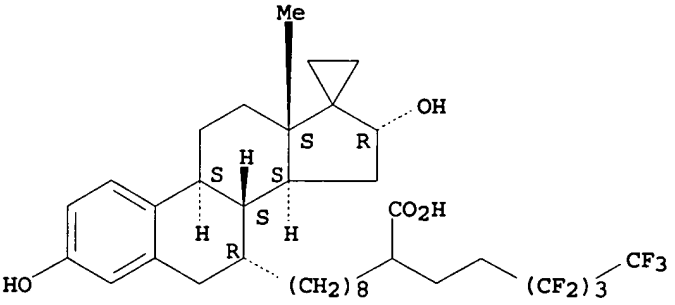
RN 862702-26-9 HCAPLUS
CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-7-undecanoic acid, 3,16-dihydroxy-α-(3,3,4,4,5,5,6,6,6-nonafluorohexyl)-, (7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



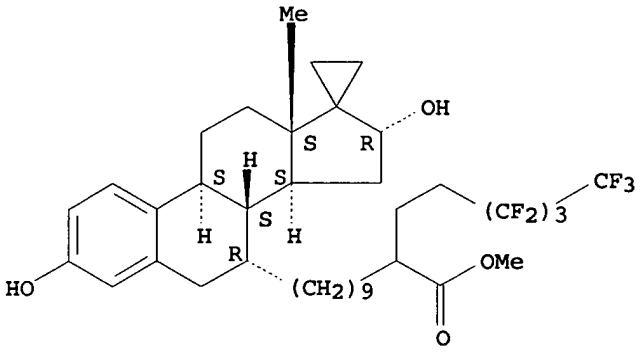
RN 862702-27-0 HCAPLUS
CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-7-decanoic acid, 3,16-dihydroxy-α-(3,3,4,4,5,5,6,6,6-nonafluorohexyl)-, (7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



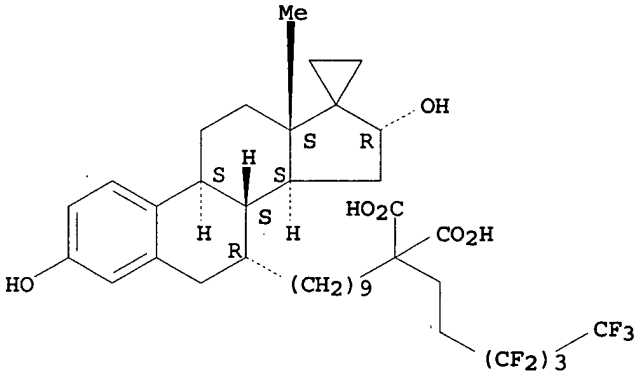
RN 862702-28-1 HCAPLUS
CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-7-undecanoic acid, 3,16-dihydroxy-α-(3,3,4,4,5,5,6,6,6-nonafluorohexyl)-, methyl ester, (7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



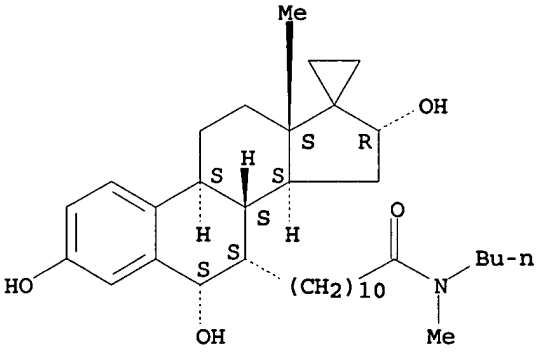
RN 862702-29-2 HCAPLUS
CN Propanedioic acid, [9-[(7α,16α)-3,16-dihydroxy-17,21-cyclo-19-norpregna-1,3,5(10)-trien-7-yl]nonyl](3,3,4,4,5,5,6,6,6-nonafluorohexyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 862702-30-5 HCAPLUS
CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-7-undecanamide, N-butyl-3,6,16-trihydroxy-N-methyl-, (6α,7α,16α)- (9CI) (CA INDEX NAME)

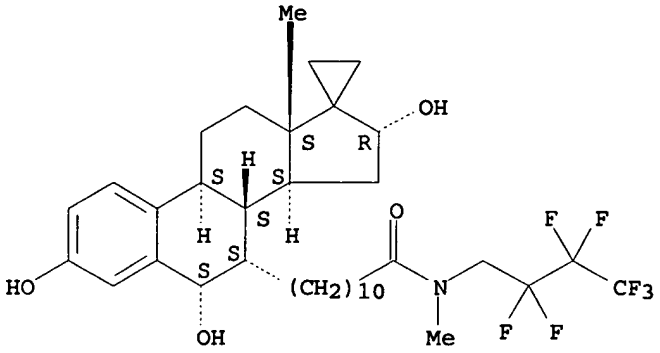
Absolute stereochemistry.



RN 862702-31-6 HCAPLUS
CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-7-undecanamide,

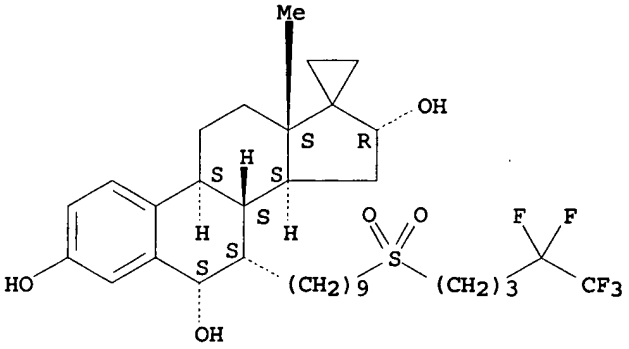
N-(2,2,3,3,4,4,4-heptafluorobutyl)-3,6,16-trihydroxy-N-methyl-,
(6α,7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



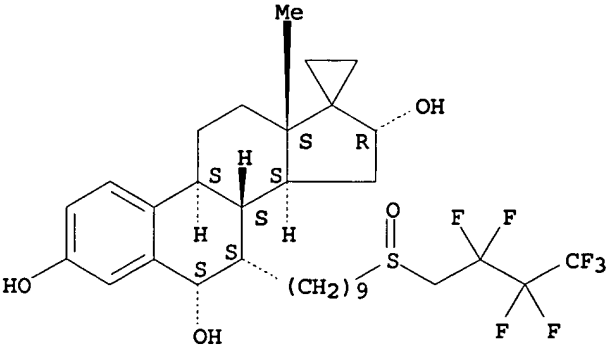
RN 862702-33-8 HCAPLUS
CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-3,6,16-triol,
7-[9-[(4,4,5,5,5-pentafluoropentyl)sulfonyl]nonyl]-,
(6α,7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



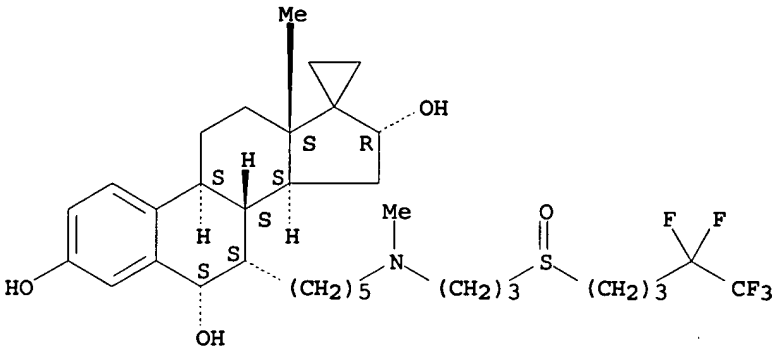
RN 862702-34-9 HCAPLUS
CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-3,6,16-triol,
7-[9-[(2,2,3,3,4,4,4-heptafluorobutyl)sulfonyl]nonyl]-,
(6α,7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



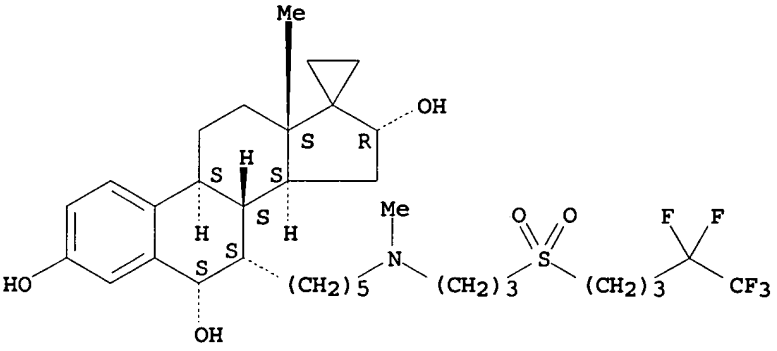
RN 862702-36-1 HCAPLUS
CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-3,6,16-triol, 7-[5-[methyl[3-[(4,4,5,5,5-pentafluoropentyl)sulfinyl]propyl]amino]pentyl]-, (6α,7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



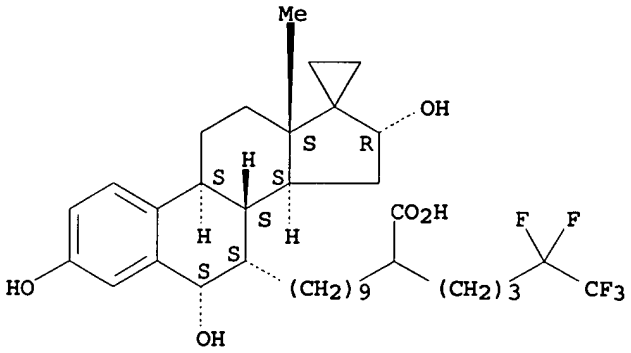
RN 862702-37-2 HCAPLUS
CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-3,6,16-triol, 7-[5-[methyl[3-[(4,4,5,5,5-pentafluoropentyl)sulfonyl]propyl]amino]pentyl]-, (6α,7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



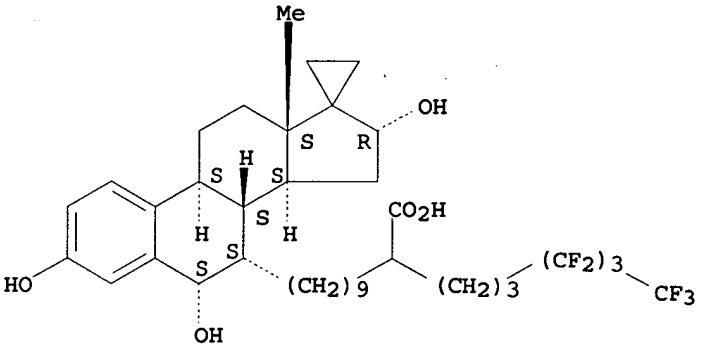
RN 862702-38-3 HCAPLUS
CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-7-undecanoic acid, 3,6,16-trihydroxy-α-(4,4,5,5,5-pentafluoropentyl)-, (6α,7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



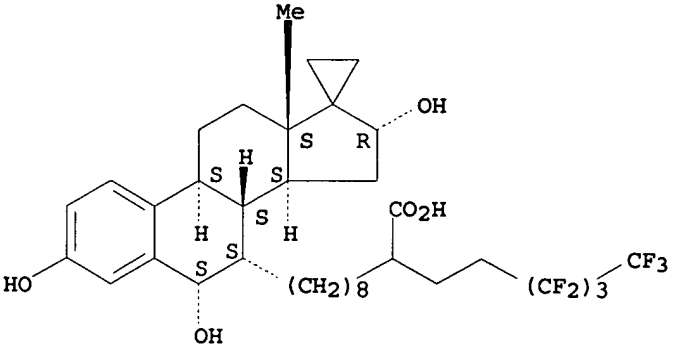
RN 862702-39-4 HCAPLUS
CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-7-undecanoic acid, 3,6,16-trihydroxy-α-(4,4,5,5,6,6,7,7,7-nonafluoroheptyl)-, (6α,7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 862702-40-7 HCAPLUS
CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-7-decanoic acid, 3,6,16-trihydroxy-α-(3,3,4,4,5,5,6,6,6-nonafluorohexyl)-, (6α,7α,16α)- (9CI) (CA INDEX NAME)

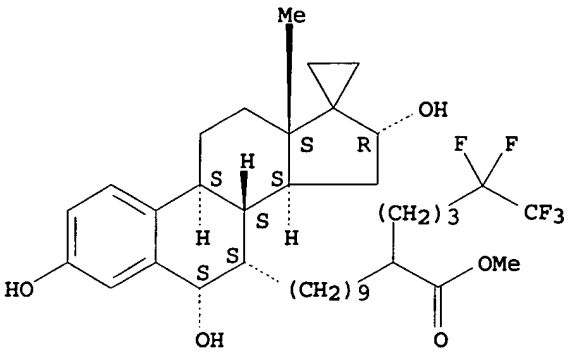
Absolute stereochemistry.



RN 862702-41-8 HCAPLUS
CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-7-undecanoic acid, 3,6,16-trihydroxy-α-(4,4,5,5,5-pentafluoropentyl)-, methyl

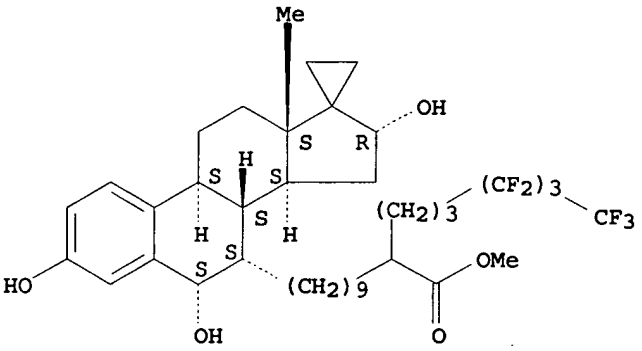
ester, (6α,7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



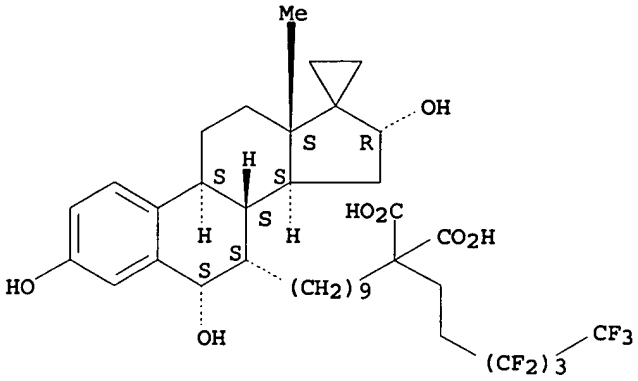
RN 862702-42-9 HCAPLUS
CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-7-undecanoic acid, 3,6,16-trihydroxy-α-(4,4,5,5,6,6,7,7,7-nonafluoroheptyl)-, methyl ester, (6α,7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



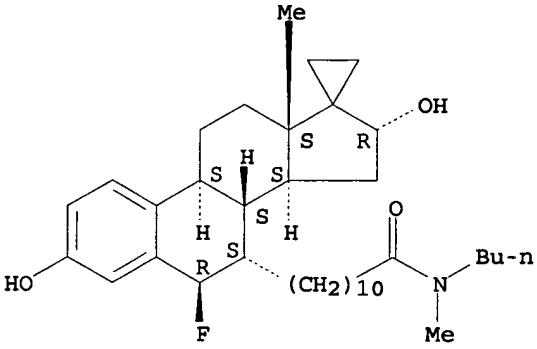
RN 862702-43-0 HCAPLUS
CN Propanedioic acid, (3,3,4,4,5,5,6,6,6-nonafluorohexyl)[9-[(6α,7α,16α)-3,6,16-trihydroxy-17,21-cyclo-19-norpregna-1,3,5(10)-trien-7-yl]nonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



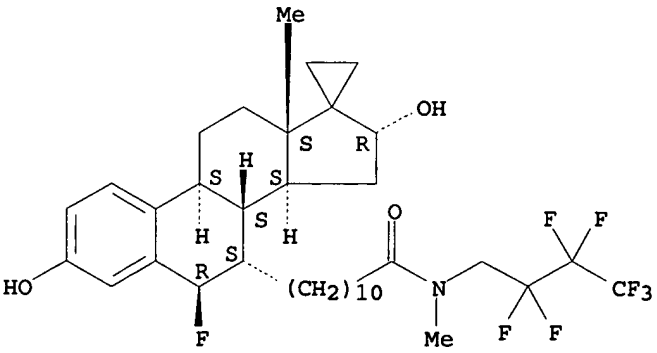
RN 862702-44-1 HCAPLUS
CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-7-undecanamide, N-butyl-6-fluoro-3,16-dihydroxy-N-methyl-, (6β,7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 862702-45-2 HCAPLUS
CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-7-undecanamide, 6-fluoro-N-(2,2,3,3,4,4,4-heptafluorobutyl)-3,16-dihydroxy-N-methyl-, (6β,7α,16α)- (9CI) (CA INDEX NAME)

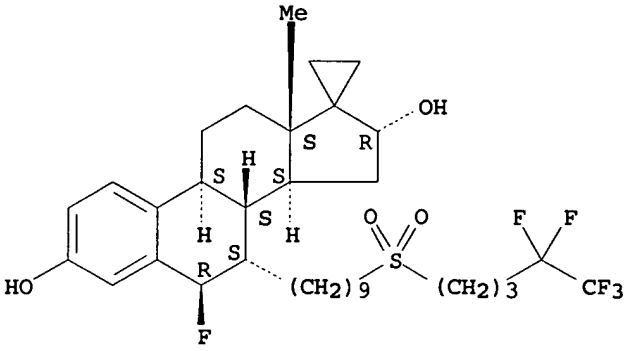
Absolute stereochemistry.



RN 862702-47-4 HCAPLUS
CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-3,16-diol,

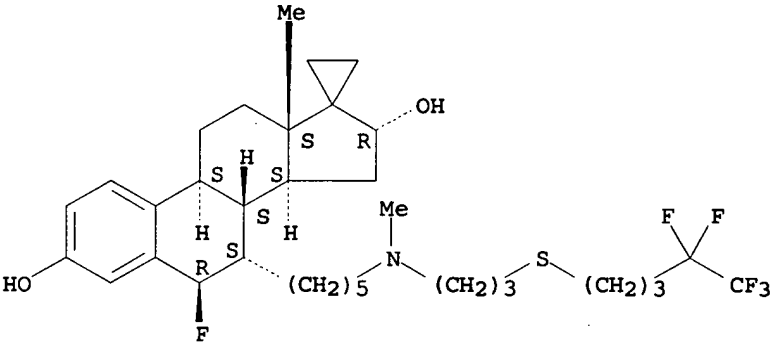
6-fluoro-7-[9-[(4,4,5,5,5-pentafluoropentyl)sulfonyl]nonyl]-, (6β,7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



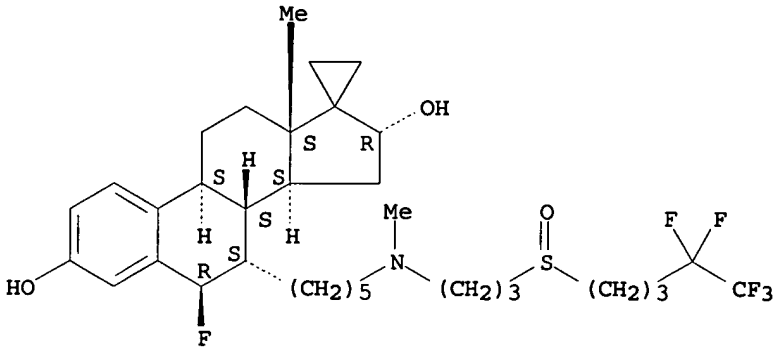
RN 862702-48-5 HCAPLUS
CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-3,16-diol, 6-fluoro-7-[5-[methyl[3-[(4,4,5,5,5-pentafluoropentyl)thio]propyl]amino]pentyl]-, (6β,7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



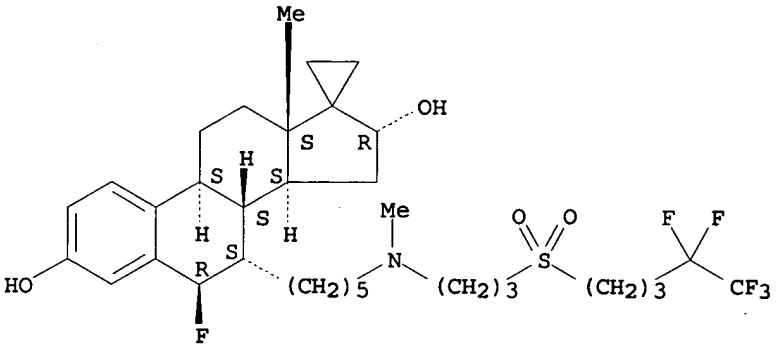
RN 862702-50-9 HCAPLUS
CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-3,16-diol, 6-fluoro-7-[5-[methyl[3-[(4,4,5,5,5-pentafluoropentyl)sulfinyl]propyl]amino]pentyl]-, (6β,7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



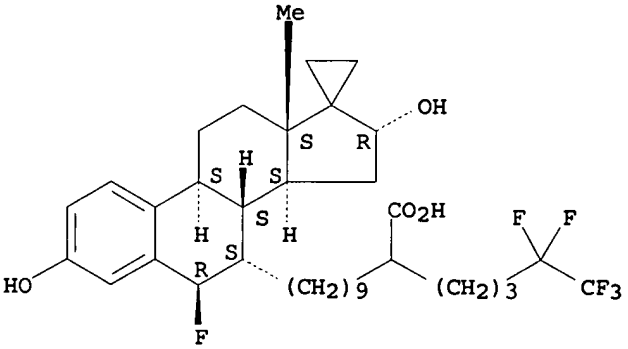
RN 862702-51-0 HCAPLUS
CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-3,16-diol, 6-fluoro-7-[5-[methyl[3-[(4,4,5,5,5-pentafluoropentyl)sulfonyl]propyl]amino]pentyl]-, (6β,7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 862702-52-1 HCAPLUS
CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-7-undecanoic acid, 6-fluoro-3,16-dihydroxy-α-(4,4,5,5,5-pentafluoropentyl)-, (6β,7α,16α)- (9CI) (CA INDEX NAME)

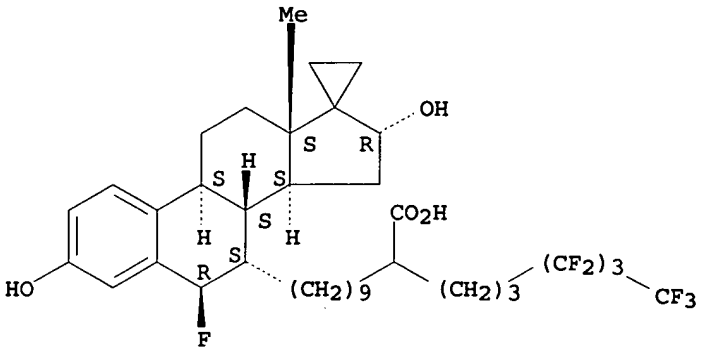
Absolute stereochemistry.



RN 862702-53-2 HCAPLUS
CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-7-undecanoic acid,

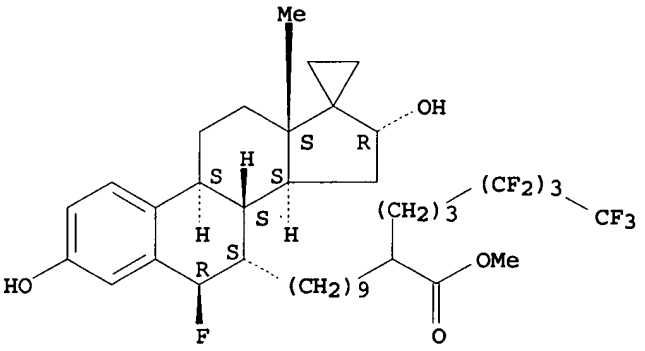
6-fluoro-3,16-dihydroxy-α-(4,4,5,5,6,6,7,7,7-nonafluoroheptyl)-, (6β,7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



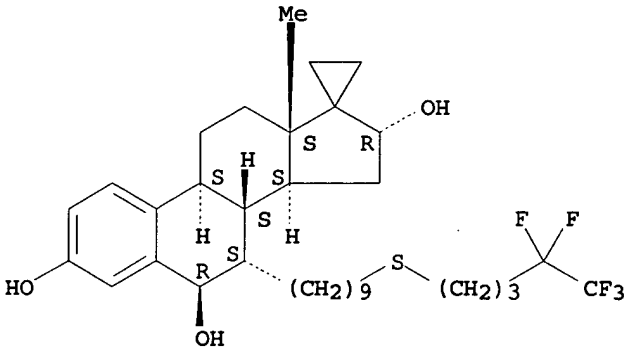
RN 862702-54-3 HCAPLUS
CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-7-undecanoic acid, 6-fluoro-3,16-dihydroxy-α-(4,4,5,5,6,6,7,7,7-nonafluoroheptyl)-, methyl ester, (6β,7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



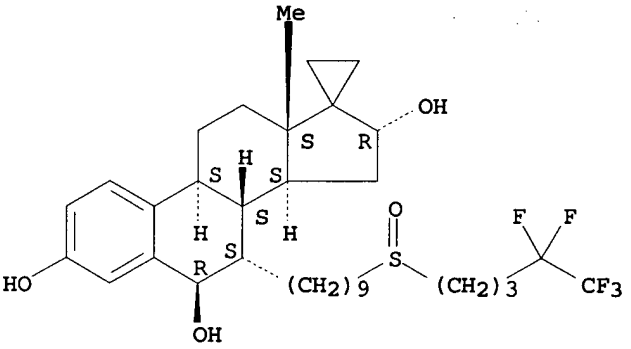
RN 862702-55-4 HCAPLUS
CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-3,6,16-triol, 7-[9-[(4,4,5,5,5-pentafluoropentyl)thio]nonyl]-, (6β,7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



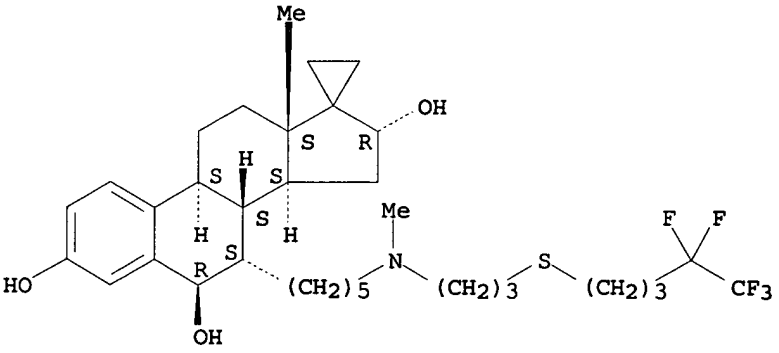
RN 862702-56-5 HCAPLUS
CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-3,6,16-triol, 7-[9-[(4,4,5,5,5-pentafluoropentyl)sulfinyl]nonyl]-, (6β,7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 862702-57-6 HCAPLUS
CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-3,6,16-triol, 7-[5-[methyl[3-[(4,4,5,5,5-pentafluoropentyl)thio]propyl]amino]pentyl]-, (6β,7α,16α)- (9CI) (CA INDEX NAME)

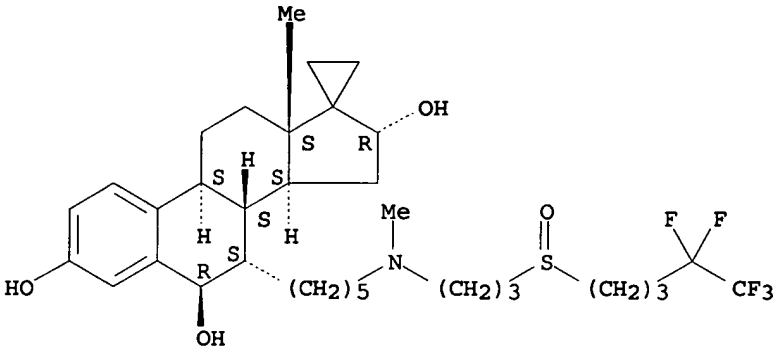
Absolute stereochemistry.



RN 862702-59-8 HCAPLUS
CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-3,6,16-triol, 7-[5-[methyl[3-[(4,4,5,5,5-pentafluoropentyl)sulfinyl]propyl]amino

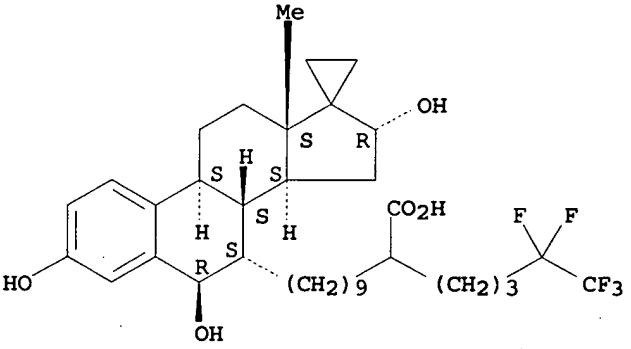
]pentyl]-, (6β,7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



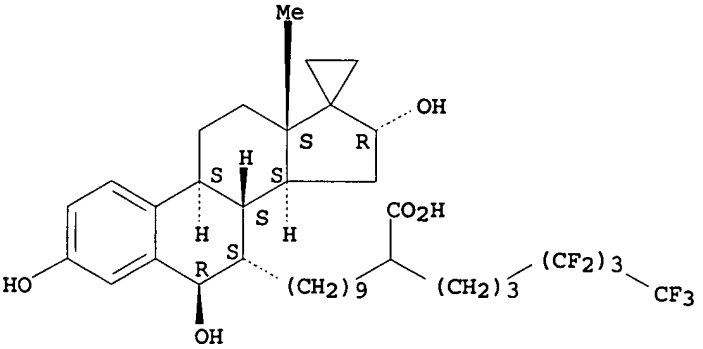
RN 862702-60-1 HCAPLUS
CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-7-undecanoic acid, 3,6,16-trihydroxy-α-(4,4,5,5,5-pentafluoropentyl)-, (6β,7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 862702-61-2 HCAPLUS
CN 17,21-Cyclo-19-norpregna-1,3,5(10)-triene-7-undecanoic acid, 3,6,16-trihydroxy-α-(4,4,5,5,6,6,7,7,7-nonafluoroheptyl)-, (6β,7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC ICM C07J003-00
CC 32-3 (**Steroids**)
Section cross-reference(s): 2, **63**
ST **estrogen** alkylene hydroxy prepn antiestrogen antitumor
IT Mammary gland, neoplasm
(**estrogen** dependent; preparation of antiestrogenic 17-alkylene-16α-hydroxyestratrienes for cancer treatment)
IT **Estrogens**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of antiestrogenic 17-alkylene-16α-hydroxyestratrienes for cancer treatment)
IT **862700-33-2P** 862700-35-4P 862700-36-5P
862700-40-1P 862700-44-5P 862700-47-8P
862700-49-0P 862700-51-4P 862700-53-6P
862700-55-8P 862700-57-0P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of antiestrogenic 17-alkylene-16α-hydroxyestratrienes for cancer treatment)
IT **862700-38-7P** 862700-42-3P **862700-46-7P**
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862700-54-7P 862700-56-9P 862700-59-2P
862701-26-6P 862701-28-8P 862701-30-2P
862701-32-4P **862701-34-6P 862701-36-8P**
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862702-61-2P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of antiestrogenic 17-alkylene-16α-hydroxyestratrienes for cancer treatment)

L53 ANSWER 3 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:1016067 HCAPLUS
DOCUMENT NUMBER: 141:424344
TITLE: Preparation of estratriene derivatives for treating asthma and airway diseases
INVENTOR(S): Stewart, Alastair George
PATENT ASSIGNEE(S): Cryptopharma Pty. Ltd., Australia; McAllister, David James; Lambert, John Nicholas
SOURCE: PCT Int. Appl., 219 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004101595	A1	20041125	WO 2004-AU630	2004 0513
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2525651	AA	20041125	CA 2004-2525651	2004 0513
EP 1625143	A1	20060215	EP 2004-732553	2004 0513
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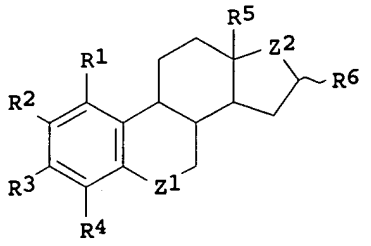
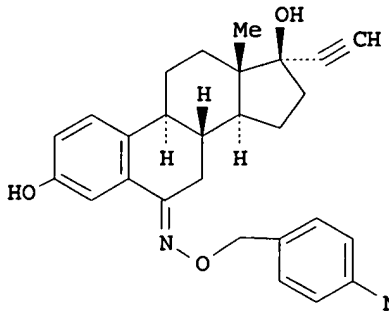
PRIORITY APPLN. INFO.:			US 2003-470379P P	2003 0513
			WO 2004-AU630 W	2004 0513

OTHER SOURCE(S): MARPAT 141:424344
GI



I



II

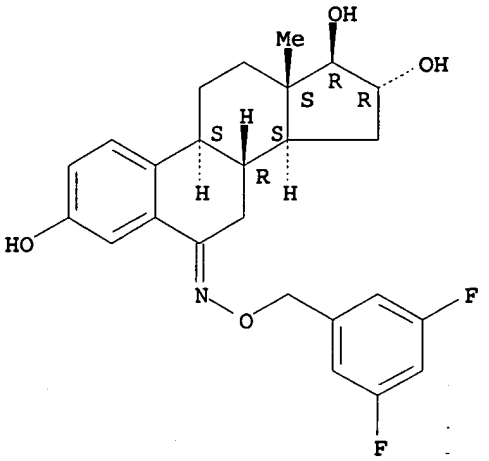
AB The present invention relates to preparation of estratriene derivs., such as I [R1, R4 = H, Ra, RcRd, CN, NO2, halo, OH, ORa, OCORa; R2 = ORb, (Rc)nARb, H, CH:NOH, OH, SRb, Rb, CN, RcRd, halo; n = 0-1; R3 = OH, ORa, RCORb, H; R5 = Me; R6 = H, OH, ORb, halo; Z1 = A, CO, CHOH, C:NOH, C:NORb, C(Rb)NRb2, CRb2, C:NNH2, C:NNRb2, O, NRb, CRbRCORb, CRbRe, CRbNRbRe, C:N-ester-Ra; Z2 = A, CO, CHOH, C:NOH, C:NORb, C(Rb)ORb, CRbRCORb, CHNRb2, CH-halo, C:N-ester-Ra; A = C:NOX, C:NORcX, C:NNHRCX, C:NNHX, C:N-ester-X; X = substituted aromatic; Ra = alkyl, cycloalkyl, alkenyl, alkynyl, aralkyl, aralkenyl, aralkynyl; Rb = H, alkyl, cycloalkyl, alkenyl, alkynyl, aralkyl, aralkenyl, aralkynyl; RC = alkylene, alkenylene, alkynylene; Rd = OH, NH2, halo, CF3, CN, CO2Ra, SRb; Re = acyl], and methods for modulating mesenchymal cell function, for instance smooth muscle and fibroblast proliferation or cytokine expression, and for treating conditions associated with mesenchymal cell function, for instance airway hyperresponsiveness associated with asthma. The prepared compds. also suppress inflammation. Thus, estratriene derivative II was prepared which at 3μM reduced basic fibroblast growth factor (bFGF) induced proliferation by 93 ± 4 %. In a preferred embodiment, the estratriene derivs. include various derivs. of 2-methoxyestradiol having a substituted aromatic substituent in the 2-, 6- or 17- position.

IT **796848-26-5P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of estratriene derivs. for treating asthma and airway diseases)

RN 796848-26-5 HCAPLUS

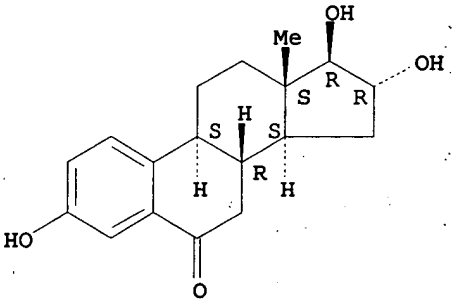
CN Estra-1,3,5(10)-trien-6-one, 3,16,17-trihydroxy-, O-[(3,5-difluorophenyl)methyl]oxime, (16α,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



IT **7323-86-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of estratriene derivs. for treating asthma and airway diseases)
RN 7323-86-6 HCAPLUS
CN Estra-1,3,5(10)-trien-6-one, 3,16,17-trihydroxy-, (16α,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC ICM C07J041-00
ICS C07J043-00; A61K031-565; A61P011-06; A61P029-00
CC 32-3 (**Steroids**)
Section cross-reference(s): **1**, 2, **63**
IT **Estrogen** receptors
Tubulins
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(preparation of estratriene derivs. and their affinity for the **estrogen** receptor and tubulin)
IT **Estrogens**
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of estratriene derivs. for treating asthma and airway diseases)
IT 94714-28-0P 796060-85-0P 796060-89-4P 796060-90-7P
796060-91-8P 796847-95-5P 796847-96-6P 796847-97-7P
796847-98-8P 796847-99-9P 796848-00-5P 796848-01-6P
796848-02-7P 796848-03-8P 796848-04-9P 796848-05-0P
796848-06-1P 796848-07-2P 796848-08-3P 796848-09-4P
796848-10-7P 796848-11-8P 796848-12-9P 796848-13-0P

796848-14-1P 796848-15-2P 796848-16-3P 796848-17-4P
796848-18-5P 796848-19-6P 796848-20-9P 796848-21-0P
796848-22-1P 796848-23-2P 796848-24-3P 796848-25-4P
796848-26-5P 796848-27-6P 796848-28-7P 796848-29-8P
796848-30-1P 796848-31-2P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of estratriene derivs. for treating asthma and airway diseases)

IT 104-81-4, 4-Methylbenzyl bromide 119-26-6, 2,4-Dinitrophenylhydrazine 362-07-2, 2-Methoxyestradiol 362-08-3, 2-Methoxyestrone 524-38-9, N-Hydroxyphthalimide 593-56-6, Methoxylamine hydrochloride 705-29-3, 3-Trifluoromethylbenzyl chloride 824-94-2, 4-Methoxybenzyl chloride 874-98-6, 3-Methoxybenzyl bromide 1944-96-3, O-(4-Nitrobenzyl)hydroxylamine 2086-26-2, O-4-Nitrobenzylhydroxylamine hydrochloride 2687-43-6, O-Benzylhydroxylamine hydrochloride 3958-60-9, 2-Nitrobenzyl bromide 6599-97-9 **7323-86-6** 7647-01-0, Hydrochloric acid, reactions 7803-49-8, Hydroxylamine, reactions 17201-43-3, 4-Cyanobenzyl bromide 21101-63-3, 4-Trifluoromethylthiobenzyl bromide 28188-41-2, 3-Cyanobenzyl bromide 38002-18-5 50824-05-0, 4-Trifluoromethoxybenzyl bromide 52552-21-3 73789-86-3, 4-Isopropylbenzyl bromide 73870-24-3, (4-Bromomethyl)pyridine hydrobromide 141776-91-2, 3,5-Difluorobenzyl bromide 159689-88-0, 3-Trifluoromethoxybenzyl bromide 796061-03-5 796061-05-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of estratriene derivs. for treating asthma and airway diseases)

REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L53 ANSWER 4 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:927229 HCAPLUS
DOCUMENT NUMBER: 141:395713
TITLE: Preparation of 8β-vinyl-11β-(ω-substituted)alkyl-estra-1,3,5(10)-trienes as ERβ antagonists
INVENTOR(S): Braeuer, Nico; Peters, Olaf; Hillisch, Alexander; Bohlmann, Rolf; Richter, Margit; Muhn, Hans Peter
PATENT ASSIGNEE(S): Schering Aktiengesellschaft, Germany
SOURCE: PCT Int. Appl., 84 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004094451	A2	20041104	WO 2004-EP4086	2004 0416
WO 2004094451	A3	20041223		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW

RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW,
AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY,
CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC,
NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM,
GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

DE 10318896	A1	20041125	DE 2003-10318896	2003 0422
CA 2522354	AA	20041104	CA 2004-2522354	2004 0416
EP 1622924	A2	20060208	EP 2004-727876	2004 0416

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE,
MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ,
EE, HU, PL, SK, HR

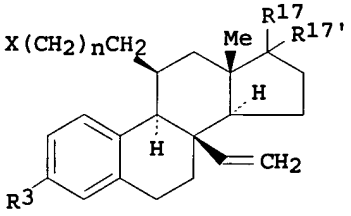
US 2005065135	A1	20050324	US 2004-829390	2004 0422

PRIORITY APPLN. INFO.:

DE 2003-10318896	A	2003 0422
US 2003-464630P	P	2003 0423
WO 2004-EP4086	W	2004 0416

OTHER SOURCE(S): MARPAT 141:395713

GI



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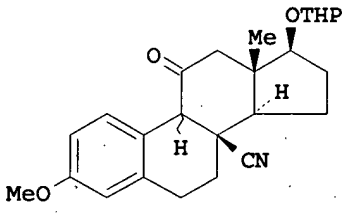
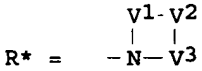


II



AB The invention relates to 8β-vinyl-11β-(ω-substituted)alkyl-estra-1,3,5(10)-trienes I [R3 = OR19, OSo2R20, OC(:O)R21; n = 3, 4, 5; X = CWYZ; Z, W = R19; WZ = O (then Y = R19, R20); R17R17' = O, CR23R24 (with R23, R24 = H, halogen); R17 = H, OR19, halogen; R17' = R19, OSO2R20, C(:O)R21, OC(:O)R21; R19 = H, CpFqHr (p = 1 - 9; q > 1 and q + r = 2p + 1), unbranched C1-8-alkyl, branched C5-6-alkyl, Ph, C3-6-cycloalkyl, (C3-6-cycloalkyl)-(C1-4-alkylene), (un)branched C2-5-alkenyl, alkynyl, (un)substituted aryl, heteroaryl, heterocycle,

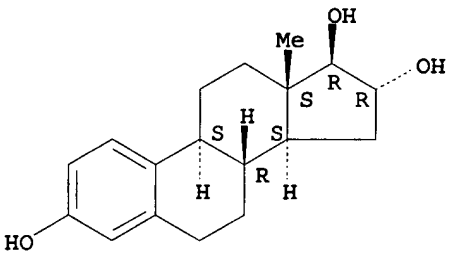
aryl-(C1-4-alkylene), heteroaryl-(C1-4-alkylene); R20 = NR21R22, CH:NOR19, R*; V1 = (CH2)m; V2 = CH2, O, S, NR25; V3 = (CH2)o; M = 0 - 8; o = 0 - 8; m + o = 2 - 12; R21, R22 = R19; R25 = R19, R20SO2, C(:O)R21], which have ERβ antagonistic activity, methods for the production thereof, the intermediate products thereof, pharmaceutical prepns. containing the inventive compds., and the use thereof for producing medicaments. Thus, I [R3 = OH, R17 = β-OH, R17' = α-H, X = CH(OH)CF3, n = 3] was prepared from estratrienone II in 10 steps. The novel compds. can be used for contraceptive purposes in men and women without influencing other **estrogen**-sensitive organs such as the uterus or the liver and while also being suitable for the treatment of benign or malignant proliferous ovarian diseases, such as ovarian carcinoma and granulosa cell tumors. The ERβ antagonistic activity of I [R3 = OH, R17 = β-OH, R17' = α-H, X = CH(OH)CF3, n = 3] was determined [EC50 = 0.8 vs. ERα (at 0.38 nM) and EC50 = 42 vs. ERβ (at 0.49 nM)].

IT **50-27-1**, Estriol
RL: PAC (Pharmacological activity); BIOL (Biological study)
(preparation of 8β-vinyl-11β-(ω-substituted)alkyl-estra-1,3,5(10)-trienes as ERβ antagonists)

RN 50-27-1 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16,17-triol, (16α,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC ICM C07J075-00

CC 32-3 (**Steroids**)
Section cross-reference(s): **1**, **2**, **63**

ST estratriene alkyl vinyl deriv prepn **estrogen** receptor beta antagonist; contraceptive male female estratriene alkyl vinyl deriv prepn; malignant proliferous ovarian disease therapeutic estratriene alkyl vinyl deriv; ovarian carcinoma therapeutic estratriene alkyl vinyl deriv; granulosa cell tumor therapeutic estratriene alkyl vinyl deriv

IT Liver
Uterus
(**estrogen**-sensitive organ, unaffected; preparation of 8β-vinyl-11β-(ω-substituted)alkyl-estra-1,3,5(10)-trienes as ERβ antagonists)

IT Antiestrogens
Estrogens
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 8β-vinyl-11β-(ω-substituted)alkyl-estra-1,3,5(10)-trienes as ERβ antagonists)

IT **Estrogen** receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(α; preparation of 8β-vinyl-11β-(ω-substituted)alkyl-estra-1,3,5(10)-trienes as ERβ antagonists)

IT **Estrogen** receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)

(β, antagonists; preparation of 8β-vinyl-11β-(ω-substituted)alkyl-estra-1,3,5(10)-trienes as ERβ antagonists)

IT **50-27-1**, Estriol 53-16-7, Estrone, biological studies
57-91-0, 17α-Estradiol 521-17-5, 5-Androstenediol
98008-06-1 367269-67-8 367269-80-5
RL: PAC (Pharmacological activity); BIOL (Biological study)
(preparation of 8β-vinyl-11β-(ω-substituted)alkyl-estra-1,3,5(10)-trienes as ERβ antagonists)

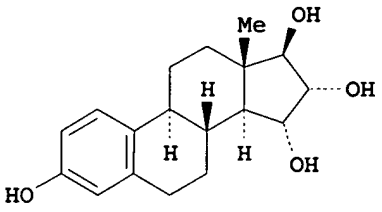
L53 ANSWER 5 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:412956 HCAPLUS
DOCUMENT NUMBER: 140:423862
TITLE: Process for preparation of estetrol from estrone derived steroids
INVENTOR(S): Verhaar, Mark Theodoor; Koch, Thomas; Warmerdan, Erwin Gerardus Jacobus
PATENT ASSIGNEE(S): Pantarhei Bioscience B.V., Neth.; Warmerdam, Erwin, Gerardus, Jacobus
SOURCE: PCT Int. Appl., 33 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004041839	A2	20040521	WO 2003-NL782	2003 1107
WO 2004041839	A3	20040701		
WO 2004041839	C1	20050721		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2505190	AA	20040521	CA 2003-2505190	2003 1107
AU 2003279624	A1	20040607	AU 2003-279624	2003 1107
EP 1562976	A2	20050817	EP 2003-772962	2003 1107
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
CN 1735627	A	20060215	CN 2003-80108518	2003 1107

PRIORITY APPLN. INFO.:		
EP 2002-79676	A	2002 1108
WO 2003-NL782	W	

2003
1107

OTHER SOURCE(S): CASREACT 140:423862; MARPAT 140:423862
GI



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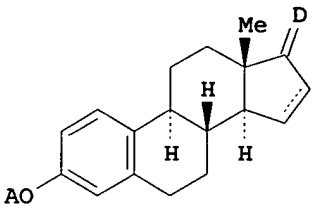


II

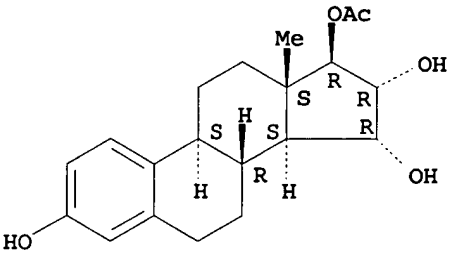
AB The present invention discloses a process for preparing estetrol (I) from estrone II (A = H, D = O, dashed bond = single bond) and estrone derived steroids, such as II [A = C1-C5 alkyl group, preferably a Me group, or a C7-C12 benzylic group, preferably a benzyl group; D = O, ethylene dioxy; dashed bond = single bond or double bond]. This process is particularly suitable to industry. The use of the prepared compds. for the manufacture of a pharmaceutical composition for hormone replacement therapy, treating or preventing a disorder from the group consisting of autoimmune diseases, breast tumors and colorectal tumors is also claimed.

IT **690996-23-7P**
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of estetrol via estrone derived steroids)

RN 690996-23-7 HCAPLUS

CN Estra-1,3,5(10)-triene-3,15,16,17-tetrol, 17-acetate, (15α,16α,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

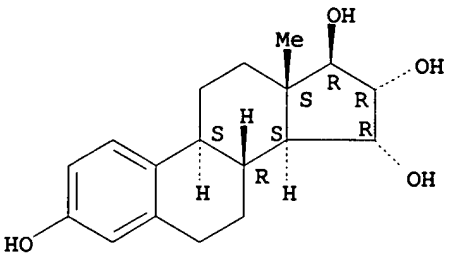


IT **15183-37-6P**, Estetrol
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(preparation of estetrol via estrone derived steroids)

RN 15183-37-6 HCAPLUS

CN Estra-1,3,5(10)-triene-3,15,16,17-tetrol, (15α,16α,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC ICM C07J001-00
CC 32-3 (**Steroids**)
Section cross-reference(s): 62, **63**
IT **Estrogens**
RL: RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of estetrol via estrone derived steroids for the manufacture of a pharmaceutical composition for use for hormone replacement therapy, treating or preventing breast tumors and colorectal tumors and promoting wound healing)
IT 138743-03-0P 534572-67-3P **690996-23-7P** 690996-24-8P
690996-25-9P 690996-26-0P 690996-27-1P
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of estetrol via estrone derived steroids)
IT **15183-37-6P**, Estetrol
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(preparation of estetrol via estrone derived steroids)

L53 ANSWER 6 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:991529 HCAPLUS
DOCUMENT NUMBER: 140:42342
TITLE: Preparation of 9α-substituted estratrienes as selectively active **estrogens**
INVENTOR(S): Kosemund, Dirk; Mueller, Gerd; Hillisch, Alexander; Fritzemeier, Karl-Heinrich; Muhn, Peter
PATENT ASSIGNEE(S): Schering Aktiengesellschaft, Germany
SOURCE: PCT Int. Appl., 45 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003104253	A2	20031218	WO 2003-EP6172	20030611
WO 2003104253	A3	20040916		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM,

AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ,
DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL,
PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN,
GQ, GW, ML, MR, NE, SN, TD, TG

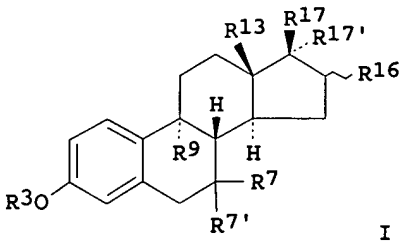
DE 10226326	A1	20040115	DE 2002-10226326	2002 0611
CA 2486495	AA	20031218	CA 2003-2486495	2003 0611
US 2004087565	A1	20040506	US 2003-458735	2003 0611
EP 1517914	A2	20050330	EP 2003-757065	2003 0611
EP 1517914	B1	20050831		

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE,
MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ,
EE, HU, SK

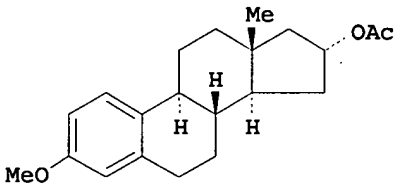
BR 2003012140	A	20050405	BR 2003-12140	2003 0611
AT 303397	E	20050915	AT 2003-757065	2003 0611
JP 2005533053	T2	20051104	JP 2004-511321	2003 0611
NO 2005000127	A	20050311	NO 2005-127	2005 0110

PRIORITY APPLN. INFO.:	DE 2002-10226326	A	2002 0611
	US 2003-443868P	P	2003 0131
	WO 2003-EP6172	W	2003 0611

OTHER SOURCE(S): MARPAT 140:42342
GI



I



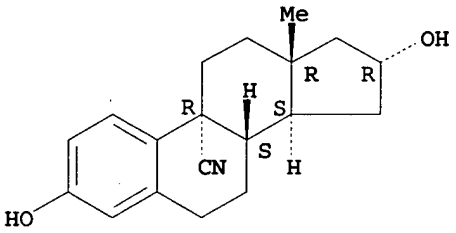
II

AB The invention relates to novel 9α-substituted estratrienes I [R3 = H, R18; R7, R7' = H, halogen; R9 = (un)branched C2-6-alkenyl (optionally partially or fully halogenated), ethynyl, prop-1-ynyl; R13 = Me, Et; R16 = OH, OR18, ; R17, R17' = H, halogen; R18 = (un)branched, (un)saturated C1-6-hydrocarbon, CF3, (un)substituted aryl, heteroaryl, aralkyl, COR19; R19 = (un)branched, (un)saturated (up to three), C1-10-hydrocarbon (optionally substituted partially or fully with halogens); R20 = NR21R22, C1-5-alkyl, C(O)R23 ; R21, R22 = H, C1-5-alkyl,C(O)R23; R23 = (un)substituted , (un)branched, (un)saturated (up to three) C1-10-hydrocarbon (optionally substituted partially or fully with halogens), C3-7-cycloalkyl, (un)substituted C4-15-cycloalkylaryl, (un)substituted aryl; NR23 = C2-6-polymethyleneimino, morpholino] as pharmaceutical active ingredients which have, in vitro, a higher affinity to **estrogen** receptor prepns. of the rat prostate than to **estrogen** receptor preparation of the rat uterus, and, in vivo, preferably a preferential action on the ovary compared to the uterus. The invention also relates to the production of said estratrienes, to the therapeutic application thereof and to pharmaceutical forms of administration containing the novel compds. Thus, 9α-vinylestra-1,3,5(10)-triene-3,16α-diol (I; R3 = R7 = R7'= R17 = R17' = H, R9 = CH:CH2, R13 = Me, R16 = α-OH) was prepared from 3-methoxyestra-1,3,5(10)-triene-16α-yl acetate (II) via regioselective and stereoselective cyanation with TMSCN in CH2Cl2 containing LiClO4 and DDQ, O-demethylation with TMSCl/NaI in MeCN, deacetylation with K2CO3 in MeOH, reduction with Dibal-H in PhMe, and Wittig reaction with MePh3PI in DMSO containing NaH. The invention further relates to the use of said compds. for treating illnesses and states related to **estrogen** deficiency. The receptor binding activity of 9α-vinylestra-1,3,5(10)-triene-3,16α-diol (I; R3 = R7 = R7'= R17 = R17' = H, R9 = CH:CH2, R13 = Me, R16 = α-OH) was determined [RBA = 1.2 (for rat uterus); RBA = 100 (for rat prostate)].

IT **634910-63-7P**, 3,16α-Dihydroxyestra-1,3,5(10)-triene-9α-carbonitrile
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and Dibal reduction of; preparation of 9α-substituted estratrienes as selectively active **estrogens**)

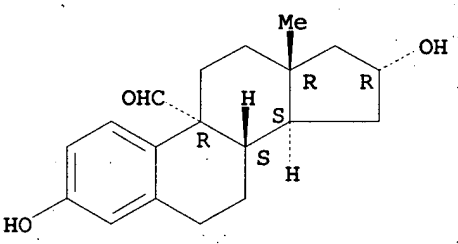
RN 634910-63-7 HCAPLUS
CN Estra-1,3,5(10)-triene-9-carbonitrile, 3,16-dihydroxy-, (16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



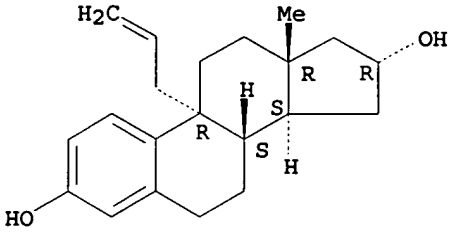
IT **634910-64-8P**, 3,16α-Dihydroxyestra-1,3,5(10)-triene-9α-carboxaldehyde
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and Wittig reactions of; preparation of 9α-substituted estratrienes as selectively active **estrogens**)
RN 634910-64-8 HCAPLUS
CN Estra-1,3,5(10)-triene-9-carboxaldehyde, 3,16-dihydroxy-, (16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



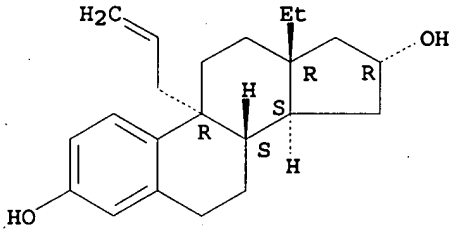
IT **634891-19-3P 634891-20-6P 634891-39-7P 634891-40-0P 634891-41-1P 634891-47-7P 634891-48-8P 634891-49-9P 634891-50-2P 634891-51-3P 634891-52-4P 634891-53-5P 634910-53-5P**, 9α-Vinylestra-1,3,5(10)-triene-3,16α-diol **634910-54-6P**, 9α-Vinyl-18a-homoestra-1,3,5(10)-triene-3,16α-diol **634910-55-7P**, 9α-(2,2-Difluorovinyl)estra-1,3,5(10)-triene-3,16α-diol **634910-56-8P**, 9α-(2,2-Difluorovinyl)-18a-homoestra-1,3,5(10)-triene-3,16α-diol **634910-57-9P**, 17β-Fluoro-9α-vinylestra-1,3,5(10)-triene-3,16α-diol **634910-58-0P**, 17,17-Difluoro-9α-vinylestra-1,3,5(10)-triene-3,16α-diol **634910-59-1P**, 9α-(1-Hexenyl)estra-1,3,5(10)-triene-3,16α-diol **634910-60-4P**, 9α-(1-Butenyl)estra-1,3,5(10)-triene-3,16α-diol
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 9α-substituted estratrienes as selectively active **estrogens**)
RN 634891-19-3 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 9-(2-propenyl)-, (16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



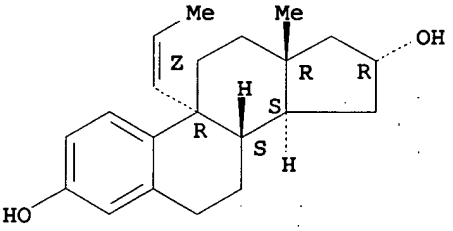
RN 634891-20-6 HCAPLUS
CN Gona-1,3,5(10)-triene-3,16-diol, 13-ethyl-9-(2-propenyl)-, (16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



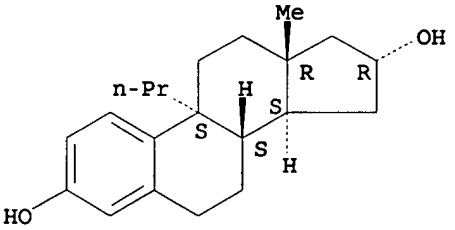
RN 634891-39-7 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 9-(1Z)-1-propenyl-, (16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 634891-40-0 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 9-propyl-, (16α)- (9CI) (CA INDEX NAME)

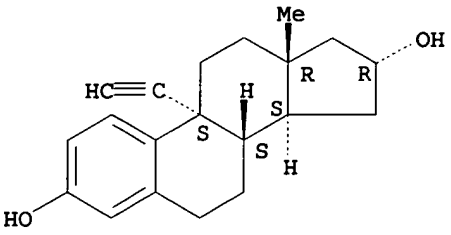
Absolute stereochemistry.



RN 634891-41-1 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 9-ethynyl-, (16α)- (9CI)

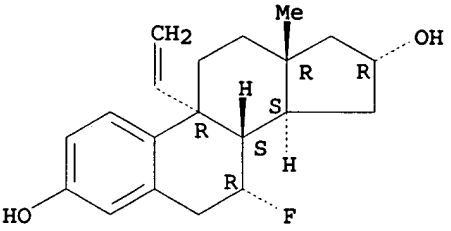
(CA INDEX NAME)

Absolute stereochemistry.



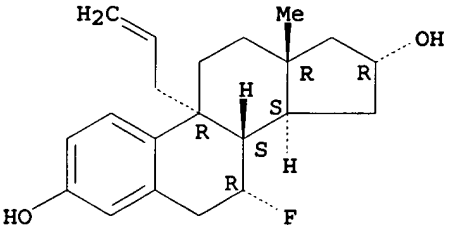
RN 634891-47-7 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 9-ethenyl-7-fluoro-, (7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



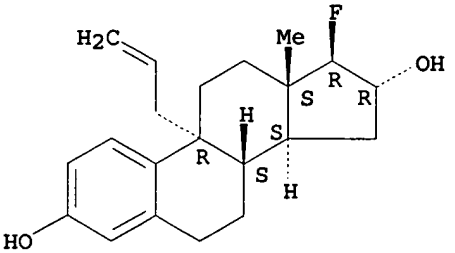
RN 634891-48-8 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 7-fluoro-9-(2-propenyl)-, (7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



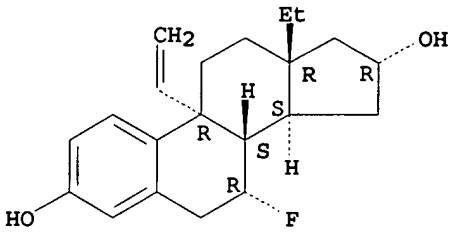
RN 634891-49-9 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 17-fluoro-9-(2-propenyl)-, (16α,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



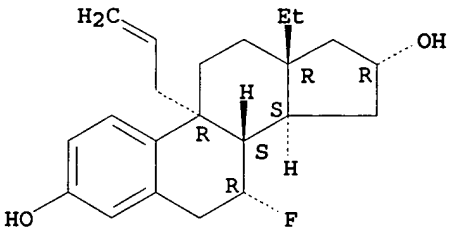
RN 634891-50-2 HCAPLUS
CN Gona-1,3,5(10)-triene-3,16-diol, 9-ethenyl-13-ethyl-7-fluoro-, (7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



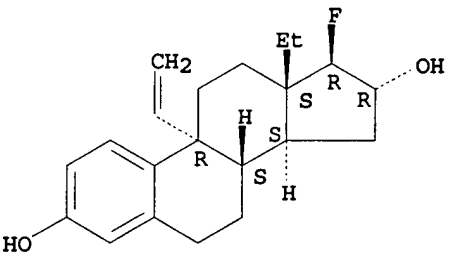
RN 634891-51-3 HCAPLUS
CN Gona-1,3,5(10)-triene-3,16-diol, 13-ethyl-7-fluoro-9-(2-propenyl)-, (7α,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



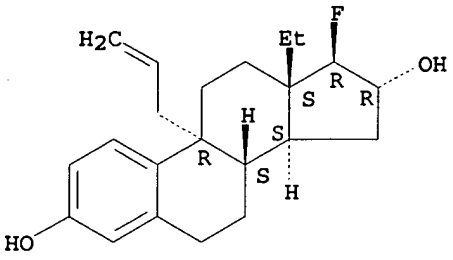
RN 634891-52-4 HCAPLUS
CN Gona-1,3,5(10)-triene-3,16-diol, 9-ethenyl-13-ethyl-17-fluoro-, (16α,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



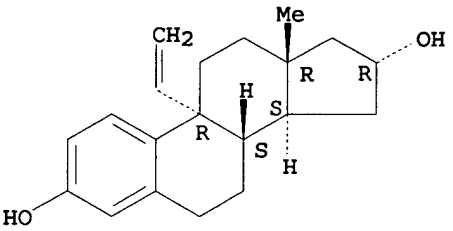
RN 634891-53-5 HCAPLUS
CN Gona-1,3,5(10)-triene-3,16-diol, 13-ethyl-17-fluoro-9-(2-propenyl)-, (16α,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



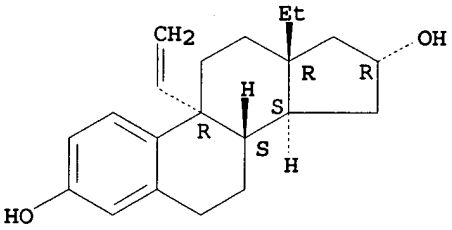
RN 634910-53-5 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 9-ethenyl-, (16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



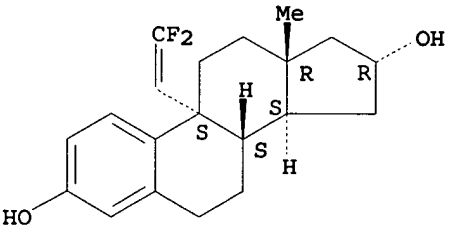
RN 634910-54-6 HCAPLUS
CN Gona-1,3,5(10)-triene-3,16-diol, 9-ethenyl-13-ethyl-, (16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 634910-55-7 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 9-(2,2-difluoroethenyl)-, (16α)- (9CI) (CA INDEX NAME)

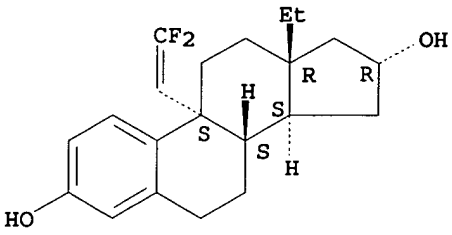
Absolute stereochemistry.



RN 634910-56-8 HCAPLUS
CN Gona-1,3,5(10)-triene-3,16-diol, 9-(2,2-difluoroethenyl)-13-ethyl-

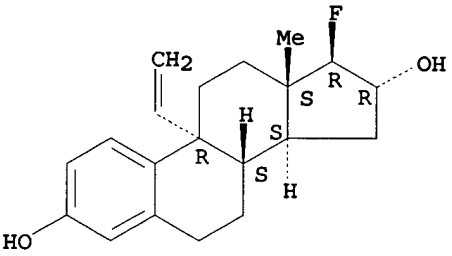
, (16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



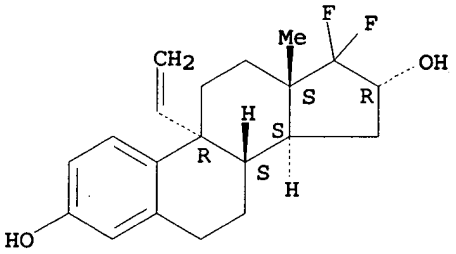
RN 634910-57-9 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 9-ethenyl-17-fluoro-, (16α,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



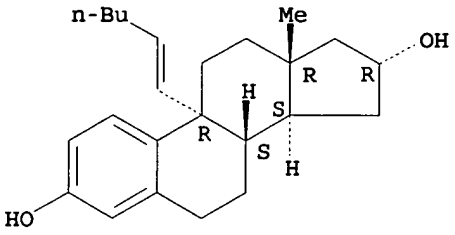
RN 634910-58-0 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 9-ethenyl-17,17-difluoro-, (16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



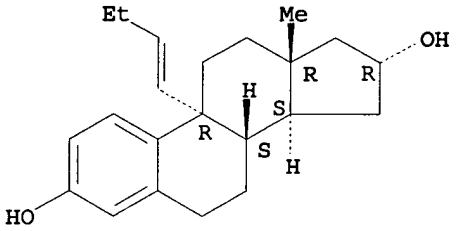
RN 634910-59-1 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 9-(1-hexenyl)-, (16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



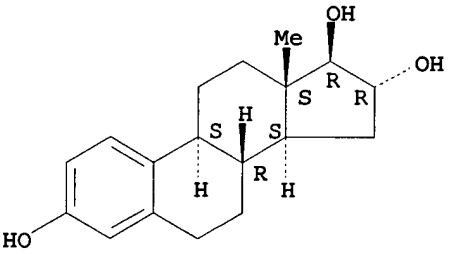
RN 634910-60-4 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, 9-(1-butenyl)-, (16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



IT **50-27-1**, Estriol
RL: PAC (Pharmacological activity); **THU (Therapeutic use)** ; BIOL (Biological study); USES (Uses)
(preparation of 9α-substituted estratrienes as selectively active **estrogens**)
RN 50-27-1 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16,17-triol, (16α,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC ICM C07J
CC 32-3 (**Steroids**)
Section cross-reference(s): **1**, **2**, **63**
ST estratriene steroid prepn **estrogenic** activity **estrogen** receptor binding
IT Steroids, preparation
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(9α-substituted estratrienes; preparation of 9α-substituted estratrienes as selectively active **estrogens**)
IT Prostate gland, disease

(benign hyperplasia, medicaments; preparation of 9α-substituted estratrienes as selectively active **estrogens**)

IT Hyperplasia
(benign prostatic, medicaments; preparation of 9α-substituted estratrienes as selectively active **estrogens**)

IT **Estrogens**
(deficiency, diseases, medicaments; preparation of 9α-substituted estratrienes as selectively active **estrogens**)

IT Hormones, animal, biological studies
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(deficiency, medicaments; preparation of 9α-substituted estratrienes as selectively active **estrogens**)

IT Circulation
Immunity
(disorder, medicaments; preparation of 9α-substituted estratrienes as selectively active **estrogens**)

IT Fertility disorders
(female, medicaments; preparation of 9α-substituted estratrienes as selectively active **estrogens**)

IT Bone, disease
(mass loss, medicaments; preparation of 9α-substituted estratrienes as selectively active **estrogens**)

IT Autoimmune disease
Hormone replacement therapy
Multiple sclerosis
Osteoporosis
Ovary, disease
Rheumatoid arthritis
(medicaments; preparation of 9α-substituted estratrienes as selectively active **estrogens**)

IT **Estrogen** receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(modulator synergism; preparation of 9α-substituted estratrienes as selectively active **estrogens**)

IT Pain
(ovarial, medicaments; preparation of 9α-substituted estratrienes as selectively active **estrogens**)

IT Analgesics
(ovary dysfunction (pain); preparation of 9α-substituted estratrienes as selectively active **estrogens**)

IT Menopause
(perimenopause, medicaments; preparation of 9α-substituted estratrienes as selectively active **estrogens**)

IT Menopause
(postmenopause, medicaments; preparation of 9α-substituted estratrienes as selectively active **estrogens**)

IT Antiarthritics
Antirheumatic agents
Bone resorption inhibitors
Cardiovascular agents
Human
(preparation of 9α-substituted estratrienes as selectively active **estrogens**)

IT Antiestrogens
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 9α-substituted estratrienes as selectively active **estrogens**)

IT 1478-53-1, Diethyl (difluoromethyl)phosphonate
RL: RCT (Reactant); RACT (Reactant or reagent)
(Horner-Emmons reaction of, with dihydroxyestratrienecarboxaldehyde; preparation of 9α-substituted estratrienes as selectively active **estrogens**)

IT 6228-47-3, Propyltriphenylphosphonium bromide 35171-55-2, Pentyltriphenylphosphonium iodide
RL: RCT (Reactant); RACT (Reactant or reagent)
(Wittig reaction of, with dihydroxyestratrienecarboxaldehyde; preparation of 9α-substituted estratrienes as selectively active **estrogens**)

IT 84449-90-1
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(**estrogen** receptor modulator co-drug; preparation of 9α-substituted estratrienes as selectively active **estrogens**)

IT **634910-63-7P**, 3,16α-Dihydroxyestra-1,3,5(10)-triene-9α-carbonitrile 634910-66-0P, 3,16α-Bis[(perhydropyran-2-yl)oxy]-18a-homoestra-1,3,5(10)-triene-9α-carbonitrile 634910-68-2P, 3,16α-Bis[(perhydropyran-2-yl)oxy]estra-1,3,5(10)-triene-9α-carbonitrile 634910-71-7P, 3,16α-Bis[(perhydropyran-2-yl)oxy]-17β-fluoroestra-1,3,5(10)-triene-9α-carbonitrile 634910-77-3P, 3,16α-Bis[(perhydropyran-2-yl)oxy]-17,17-difluoroestra-1,3,5(10)-triene
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and Dibal reduction of; preparation of 9α-substituted estratrienes as selectively active **estrogens**)

IT 634910-61-5P, 9α-Cyano-3-methoxyestra-1,3,5(10)-trien-16α-yl acetate
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and O-demethylation of; preparation of 9α-substituted estratrienes as selectively active **estrogens**)

IT **634910-64-8P**, 3,16α-Dihydroxyestra-1,3,5(10)-triene-9α-carboxaldehyde 634910-67-1P, 3,16α-Dihydroxy-18a-homoestra-1,3,5(10)-triene-9α-carboxaldehyde 634910-69-3P 634910-72-8P, 3,16α-Dihydroxy-17β-fluoroestra-1,3,5(10)-triene-9α-carboxaldehyde 634910-74-0P, 3,16α-Bis[(perhydropyran-2-yl)oxy]-17,17-difluoroestra-1,3,5(10)-triene-9α-carboxaldehyde
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and Wittig reactions of; preparation of 9α-substituted estratrienes as selectively active **estrogens**)

IT 634910-62-6P, 9α-Cyano-3-hydroxyestra-1,3,5(10)-trien-16α-yl acetate
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and deacetylation of; preparation of 9α-substituted estratrienes as selectively active **estrogens**)

IT **634891-19-3P 634891-20-6P** 634891-21-7P
634891-22-8P 634891-23-9P 634891-25-1P 634891-26-2P
634891-27-3P 634891-28-4P 634891-29-5P 634891-30-8P
634891-31-9P 634891-32-0P 634891-33-1P 634891-34-2P
634891-35-3P 634891-36-4P 634891-37-5P 634891-38-6P
634891-39-7P 634891-40-0P 634891-41-1P
634891-42-2P 634891-43-3P 634891-44-4P 634891-45-5P
634891-46-6P **634891-47-7P 634891-48-8P**
634891-49-9P 634891-50-2P 634891-51-3P
634891-52-4P 634891-53-5P 634910-53-5P
, 9α-Vinylestra-1,3,5(10)-triene-3,16α-diol
634910-54-6P, 9α-Vinyl-18a-homoestra-1,3,5(10)-triene-3,16α-diol **634910-55-7P**, 9α-(2,2-Difluorovinyl)estra-1,3,5(10)-triene-3,16α-diol **634910-56-8P**, 9α-(2,2-Difluorovinyl)-18a-homoestra-1,3,5(10)-triene-3,16α-diol **634910-57-9P**, 17β-Fluoro-9α-vinylestra-1,3,5(10)-triene-3,16α-diol **634910-58-0P**, 17,17-Difluoro-9α-vinylestra-

1,3,5(10)-triene-3,16α-diol **634910-59-1P**, 9α-(1-Hexenyl)estra-1,3,5(10)-triene-3,16α-diol **634910-60-4P**, 9α-(1-Butenyl)estra-1,3,5(10)-triene-3,16α-diol
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 9α-substituted estratrienes as selectively active **estrogens**)

IT **50-27-1**, Estriol 50-28-2, Estradiol, biological studies 53-16-7, Estrone, biological studies 57-91-0, 17α-Estradiol 446-72-0, Genistein 479-13-0, Coumestrol 521-17-5, 5-Androstenediol
RL: PAC (Pharmacological activity); **THU (Therapeutic use)**; BIOL (Biological study); USES (Uses)
(preparation of 9α-substituted estratrienes as selectively active **estrogens**)

IT 76820-87-6, 3-Methoxyestra-1,3,5(10)-trien-16α-yl acetate 634910-65-9, 3,16α-Bis[(perhydropyran-2-yl)oxy]-18a-homoestra-1,3,5(10)-triene 634910-70-6, 3,16α-Bis[(perhydropyran-2-yl)oxy]-17β-fluoroestra-1,3,5(10)-triene 634910-73-9, 3,16α-Bis[(perhydropyran-2-yl)oxy]-17,17-difluoroestra-1,3,5(10)-triene-9α-carbonitrile 634910-75-1, 3,16α-Bis[(perhydropyran-2-yl)oxy]estra-1,3,5(10)-triene
RL: RCT (Reactant); RACT (Reactant or reagent)
(regioselective and stereoselective cyanation of; preparation of 9α-substituted estratrienes as selectively active **estrogens**)

L53 ANSWER 7 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:777821 HCAPLUS
DOCUMENT NUMBER: 139:292396
TITLE: Preparation and anti-**estrogen** effect of 19-nor-17α-pregna-1,3,5(10)-trien-17β-ols with a 21,16α-lactone ring substituted with a long chain at the 11β position
INVENTOR(S): Mueller, Gerd; Hillisch, Alexander; Hoffmann, Jens; Fritzemeier, Karl-Heinrich
PATENT ASSIGNEE(S): Schering Aktiengesellschaft, Germany
SOURCE: PCT Int. Appl., 27 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003080641	A1	20031002	WO 2003-EP3226	2003 0327

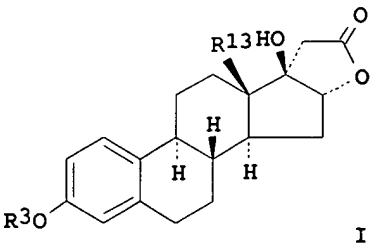
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

DE 10214180	A1	20031016	DE 2002-10214180	2002 0327
AU 2003221528	A1	20031008	AU 2003-221528	2003 0327
US 2003229059	A1	20031211	US 2003-397854	2003 0327
US 2004014735	A1	20040122	US 2003-397855	2003 0327
US 6956031	B2	20051018		
EP 1490391	A1	20041229	EP 2003-717244	2003 0327
EP 1490391	B1	20051221		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2005526805	T2	20050908	JP 2003-578394	2003 0327
AT 313552	E	20060115	AT 2003-717244	2003 0327

PRIORITY APPLN. INFO.:	DE 2002-10214180	A	2002 0327
	US 2002-374516P	P	2002 0423
	US 2002-374517P	P	2002 0423
	DE 2002-10214179	A	2002 0327
	WO 2003-EP3226	W	2003 0327

OTHER SOURCE(S): MARPAT 139:292396

GI



I

AB The invention relates to novel 19-nor-17α-pregna-1,3,5(10)-trien-17β-ols with a 21,16α-lactone ring and a long chain substituent in the 11β position, e.g., I [R3 =

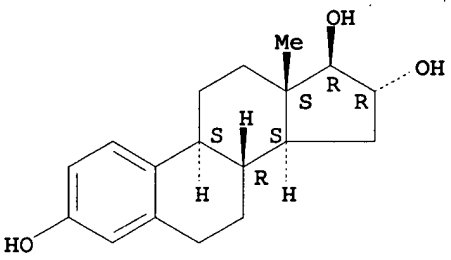
C1-4-alkyl, C2-6-acyl, ; R11 = straight chain C6-17 alkyl group; R13 = Me, Et; R18 = NR19R20; R19, R20 = H, C1-5-alkyl, C(:O)R21; R21 =]. Thus, I [R3 = H, R11 = hexyl, R13 = Me] was prepared from 11β-hexyl-17-oxoestra-1,3,5(10)-triene-3,16α-diyl diacetate via condensation with acetonitrile lithium salt. The compds. have a tissue-selective pure anti-**estrogen** effect and are thus suitable for the production of medicaments. The **estrogen** receptor binding activity of was determined [RBA = 26.2 vs. rat uterus; RBA = 1.2 vs. rat prostate]; inhibition of MCF-7 mammary carcinoma cells by I [R3 = H, R11 = hexyl, R13 = Me] (at 1x10-5 M) was also determined

IT **50-27-1**, Estriol
RL: PAC (Pharmacological activity); BIOL (Biological study)
(**estrogen** receptor binding activity of; preparation and anti-**estrogen** effect of 19-nor-17α-pregna-1,3,5(10)-trien-17β-ols 11β-alkyl 21,16α-lactone ring derivs.)

RN 50-27-1 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16,17-triol, (16α,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC ICM C07J001-00
ICS A61K031-585; A61P035-00

CC 32-5 (**Steroids**)
Section cross-reference(s): **1**, 2, **63**

ST pregnane nor sterol lactone deriv antiestrogen antitumor; norpregnatrienediol lactone prepn **estrogen** receptor binding antiproliferative activity

IT **Estrogen** receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(binding activity; preparation and anti-**estrogen** effect of 19-nor-17α-pregna-1,3,5(10)-trien-17β-ols 11β-alkyl 21,16α-lactone ring derivs.)

IT Mammary gland, neoplasm
Prostate gland, neoplasm
(carcinoma, medicaments; preparation and anti-**estrogen** effect of 19-nor-17α-pregna-1,3,5(10)-trien-17β-ols 11β-alkyl 21,16α-lactone ring derivs.)

IT Carcinoma
(endometrial, medicaments; preparation and anti-**estrogen** effect of 19-nor-17α-pregna-1,3,5(10)-trien-17β-ols 11β-alkyl 21,16α-lactone ring derivs.)

IT Uterus, neoplasm
(endometrium, carcinoma, medicaments; preparation and anti-**estrogen** effect of 19-nor-17α-pregna-1,3,5(10)-trien-17β-ols 11β-alkyl 21,16α-lactone ring derivs.)

IT Carcinoma
(mammary, medicaments; preparation and anti-**estrogen** effect of 19-nor-17α-pregna-1,3,5(10)-trien-17β-ols 11β-alkyl 21,16α-lactone ring derivs.)

IT Sterols

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(norsterols; preparation and anti-**estrogen** effect of 19-nor-17α-pregna-1,3,5(10)-trien-17β-ols 11β-alkyl 21,16α-lactone ring derivs.)

IT Antitumor agents
Human
(preparation and anti-**estrogen** effect of 19-nor-17α-pregna-1,3,5(10)-trien-17β-ols 11β-alkyl 21,16α-lactone ring derivs.)

IT Antiestrogens
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and anti-**estrogen** effect of 19-nor-17α-pregna-1,3,5(10)-trien-17β-ols 11β-alkyl 21,16α-lactone ring derivs.)

IT Carcinoma
(prostatic, medicaments; preparation and anti-**estrogen** effect of 19-nor-17α-pregna-1,3,5(10)-trien-17β-ols 11β-alkyl 21,16α-lactone ring derivs.)

IT 608101-30-0, 11β-Hexyl-17-oxoestra-1,3,5(10)-triene-3,16α-diyl diacetate 608101-31-1, 11β-Octyl-17-oxoestra-1,3,5(10)-triene-3,16α-diyl diacetate 608101-32-2, 11β-Decyl-17-oxoestra-1,3,5(10)-triene-3,16α-diyl diacetate 608101-33-3, 11β-Dodecyl-17-oxoestra-1,3,5(10)-triene-3,16α-diyl diacetate
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation with acetonitrile lithium salt; preparation and anti-**estrogen** effect of 19-nor-17α-pregna-1,3,5(10)-trien-17β-ols 11β-alkyl 21,16α-lactone ring derivs.)

IT **50-27-1**, Estriol 50-28-2, Estradiol, biological studies 53-16-7, Estrone, biological studies 57-91-0, 17α-Estradiol 446-72-0, Genistein 479-13-0, Coumestrol 521-17-5, 5-Androstenediol
RL: PAC (Pharmacological activity); BIOL (Biological study)
(**estrogen** receptor binding activity of; preparation and anti-**estrogen** effect of 19-nor-17α-pregna-1,3,5(10)-trien-17β-ols 11β-alkyl 21,16α-lactone ring derivs.)

IT 608101-26-4P, 3,17β-Dihydroxy-11β-hexyl-19-nor-17α-pregna-1,3,5(10)-triene-21,16α-lactone 608101-27-5P, 3,17β-Dihydroxy-11β-octyl-19-nor-17α-pregna-1,3,5(10)-triene-21,16α-lactone 608101-28-6P, 3,17β-Dihydroxy-11β-decyl-19-nor-17α-pregna-1,3,5(10)-triene-21,16α-lactone 608101-29-7P, 3,17β-Dihydroxy-11β-dodecyl-19-nor-17α-pregna-1,3,5(10)-triene-21,16α-lactone
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and **estrogen** receptor binding activity of; preparation and anti-**estrogen** effect of 19-nor-17α-pregna-1,3,5(10)-trien-17β-ols 11β-alkyl 21,16α-lactone ring derivs.)

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

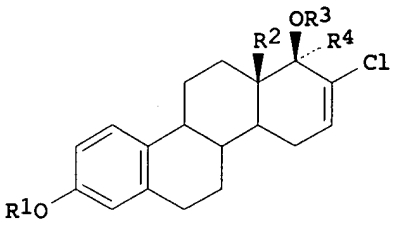
L53 ANSWER 8 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:331993 HCAPLUS
DOCUMENT NUMBER: 138:354135
TITLE: Preparation of 17-chloro-D-homosteroid as selective **estrogen** receptor

antagonists
INVENTOR(S): Tornus, Ingo; Ring, Sven; Schubert, Gerd
PATENT ASSIGNEE(S): Schering AG, Germany
SOURCE: Ger. Offen., 12 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10151365	A1	20030430	DE 2001-10151365	2001 1017
WO 2002068548	A1	20020906	WO 2002-EP2117	2002 0227
WO 2002068548	C2	20030220		
WO 2002068548	A3	20030605		
WO 2002068548	C1	20031224		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2003083377	A1	20030501	US 2002-83685	2002 0227
US 6794409	B2	20040921		
EP 1365768	A2	20031203	EP 2002-706750	2002 0227
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2004529107	T2	20040924	JP 2002-568649	2002 0227
US 2005020695	A1	20050127	US 2004-909540	2004 0803

PRIORITY APPLN. INFO.:		
US 2001-271409P	P	2001 0227
DE 2001-10151365	A	2001 1017
US 2001-329736P	P	2001 1018
US 2002-83685	A3	2002 0227
WO 2002-EP2117	W	2002

OTHER SOURCE(S): CASREACT 138:354135; MARPAT 138:354135
GI



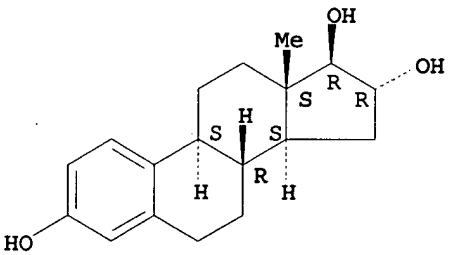
AB The present invention discloses preparation of 17-chloro-D-homosteroids, e.g., I [R1 = H, C1-6-alkanoyl, COPh; R2 = C1-6-alkyl; R3 = H, C1-6-alkyl, C1-6-alkanoyl, COPh; R4 = H, C1-6-alkyl, fluoroalkyl, C.tplbond.CR5; R5 = H, C1-6-alkyl, (un)substituted phenyl], for their use as selective **estrogen** receptor antagonists. Thus, I [R1 = R3 = H, R2 = Et, R4 = CH2C.tplbond.CH] was prepared from 3-methoxy-18a-homoestra-1,3,5(10)-trien-17β-ol via Jones oxidation, enol silylation, ring expansion with sodium trichloroacetate,. The new compds. are suitable for contraception with men and women, without affecting other **estrogenic**-sensitive organs like the uterus or the liver. They are also suitable for the treatment of benign or malignant proliferative illnesses of the ovaries, like ovarian carcinomas and Granulosa cell tumors.

IT **50-27-1**, Estriol
RL: PAC (Pharmacological activity); **THU (Therapeutic use)**; BIOL (Biological study); USES (Uses)
(preparation of 17-chloro-D-homosteroids as selective **estrogen** receptor antagonists)

RN 50-27-1 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16,17-triol, (16α,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC ICM C07J063-00
ICS A61K031-565

CC 32-3 (**Steroids**)
Section cross-reference(s): **1**, **2**, **63**

ST homosteroid chloro prepn **estrogen** receptor antagonist; ovary proliferative illness treatment chlorohomosteroid; ovarian carcinoma treatment chlorohomosteroid; Granulosa cell tumor treatment chlorohomosteroid

IT Coupling reaction
(Sonagashira; preparation of 17-chloro-D-homosteroids as selective **estrogen** receptor antagonists)

IT Progesterone receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(antagonist; preparation of 17-chloro-D-homosteroids as selective **estrogen** receptor antagonists)
IT **Estrogen** receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(antagonists; preparation of 17-chloro-D-homosteroids as selective **estrogen** receptor antagonists)
IT Ovulation
(control; preparation of 17-chloro-D-homosteroids as selective **estrogen** receptor antagonists)
IT Contraceptives
(female; preparation of 17-chloro-D-homosteroids as selective **estrogen** receptor antagonists)
IT Ovary
(follicle cell, early genesis, promotion; preparation of 17-chloro-D-homosteroids as selective **estrogen** receptor antagonists)
IT Ovary, neoplasm
(granulosa cell, treatment; preparation of 17-chloro-D-homosteroids as selective **estrogen** receptor antagonists)
IT Contraceptives
(male; preparation of 17-chloro-D-homosteroids as selective **estrogen** receptor antagonists)
IT Progestogens
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(mesoprogestins; preparation of 17-chloro-D-homosteroids as selective **estrogen** receptor antagonists)
IT Organometallic compounds
RL: RGT (Reagent); RACT (Reactant or reagent)
(organolithium reaction with acetylene or its alkyl or aryl derivs.; preparation of 17-chloro-D-homosteroids as selective **estrogen** receptor antagonists)
IT Silanes
RL: RCT (Reactant); RACT (Reactant or reagent)
(organosilanes, with 17-chloro-D-homoestrone; preparation of 17-chloro-D-homosteroids as selective **estrogen** receptor antagonists)
IT Human
(preparation of 17-chloro-D-homosteroids as selective **estrogen** receptor antagonists)
IT **Estrogens**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 17-chloro-D-homosteroids as selective **estrogen** receptor antagonists)
IT Ovary, disease
(proliferative, treatment; preparation of 17-chloro-D-homosteroids as selective **estrogen** receptor antagonists)
IT Grignard reagents
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with 17-chloro-D-homoestrone; preparation of 17-chloro-D-homosteroids as selective **estrogen** receptor antagonists)
IT Ovary, neoplasm
(treatment; preparation of 17-chloro-D-homosteroids as selective **estrogen** receptor antagonists)
IT 3625-82-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(Jones oxidation of; preparation of 17-chloro-D-homosteroids as selective **estrogen** receptor antagonists)
IT 454485-63-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(O-demethylation of; preparation of 17-chloro-D-homosteroids as selective **estrogen** receptor antagonists)

IT 9034-40-6, GnRH
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(antagonists; preparation of 17-chloro-D-homosteroids as selective **estrogen** receptor antagonists)
IT 865-47-4
RL: RGT (Reagent); RACT (Reactant or reagent)
(deprotonation by, of acetylene in reaction with 17-chloro-D-homoestrone; preparation of 17-chloro-D-homosteroids as selective **estrogen** receptor antagonists)
IT 1624-62-0, 3-Methoxyestra-1,3,5(10)-trien-17-one
RL: RCT (Reactant); RACT (Reactant or reagent)
(enol silylation of; preparation of 17-chloro-D-homosteroids as selective **estrogen** receptor antagonists)
IT 454485-57-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation and O-demethylation of; preparation of 17-chloro-D-homosteroids as selective **estrogen** receptor antagonists)
IT 454485-55-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and O-demethylation of; preparation of 17-chloro-D-homosteroids as selective **estrogen** receptor antagonists)
IT 454485-60-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and desilylation of; preparation of 17-chloro-D-homosteroids as selective **estrogen** receptor antagonists)
IT 848-04-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and enol silylation of; preparation of 17-chloro-D-homosteroids as selective **estrogen** receptor antagonists)
IT 454485-56-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with alkynylmagnesium bromides; preparation of 17-chloro-D-homosteroids as selective **estrogen** receptor antagonists)
IT 454485-58-6P, 17-Chloro-3-methoxy-17a-homoestra-1,3,5(10),16-tetraen-17a-one
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and reaction of, with methylmagnesium bromide or (trifluoromethyl)trimethylsilane; preparation of 17-chloro-D-homosteroids as selective **estrogen** receptor antagonists)
IT 454485-61-1P 454485-62-2P 454485-64-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and reductive demethylation of; preparation of 17-chloro-D-homosteroids as selective **estrogen** receptor antagonists)
IT 115419-13-1P, 3-Methoxy-17-[(trimethylsilyl)oxy]estra-1,3,5(10)-triene 518045-87-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and ring expansion of, with sodium trichloroacetate; preparation of 17-chloro-D-homosteroids as selective **estrogen** receptor antagonists)
IT 454485-33-7P 454485-34-8P 454485-36-0P 454485-37-1P
454485-38-2P 454485-39-3P 454485-40-6P 454485-41-7P
454485-42-8P 454485-43-9P 454485-44-0P 454485-45-1P
454485-46-2P 454485-47-3P 454485-48-4P 454485-49-5P
454485-52-0P 454485-53-1P 454485-54-2P 518045-83-5P
518045-85-7P 518045-86-8P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of 17-chloro-D-homosteroids as selective **estrogen** receptor antagonists)

IT **50-27-1**, Estriol 50-28-2, Estradiol, biological studies 53-16-7, Estrone, biological studies 57-91-0, 17α-Estradiol 446-72-0, Genistein 479-13-0, Coumestrol 521-17-5, 5-Androstene-diol
RL: PAC (Pharmacological activity); **THU (Therapeutic use)** ; BIOL (Biological study); USES (Uses)
(preparation of 17-chloro-D-homosteroids as selective **estrogen** receptor antagonists)

IT 354-64-3, Pentafluoroethyliodide 3466-32-8, 4-Bromophenylmethylsulfone 4301-14-8, Ethynylmagnesium bromide 16466-97-0, (1-Propynyl)magnesium bromide
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of 17-chloro-D-homosteroids as selective **estrogen** receptor antagonists)

IT 74-86-2, Acetylene, reactions 81290-20-2, (Trifluoromethyl)trimethylsilane
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with 17-chloro-D-homoestrone; preparation of 17-chloro-D-homosteroids as selective **estrogen** receptor antagonists)

IT 91935-83-0, Pentafluoroethyllithium
RL: RGT (Reagent); RACT (Reactant or reagent)
(reaction of, with 17-chloro-D-homoestrone; preparation of 17-chloro-D-homosteroids as selective **estrogen** receptor antagonists)

IT 650-51-1, Sodium trichloroacetate
RL: RCT (Reactant); RACT (Reactant or reagent)
(ring expansion of 3-methoxy-18a-homoestra-1,3,5(10)-trien-17-one enol silyl ether with; preparation of 17-chloro-D-homosteroids as selective **estrogen** receptor antagonists)

L53 ANSWER 9 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:298714 HCAPLUS
DOCUMENT NUMBER: 138:304438
TITLE: Preparation of 8β-substituted 11β-(para-substituted)aryl-estra-2,3,5(10)-triene derivatives as contraceptives and antiproliferatives
INVENTOR(S): Braeuer, Nico; Peters, Olaf; Hillisch, Alexander; Hegele-hartung, Christa; Muhn, Peter
PATENT ASSIGNEE(S): Schering AG, Germany
SOURCE: Ger. Offen., 18 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10151114	A1	20030417	DE 2001-10151114	2001 1015
WO 2003033516	A1	20030424	WO 2002-EP11533	2002 1015

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN,

YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

US 2003171345	A1	20030911	US 2002-270077	2002 1015
PRIORITY APPLN. INFO.:			DE 2001-10151114	A 2001 1015
			US 2001-330728P	P 2001 1029

OTHER SOURCE(S): MARPAT 138:304438
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

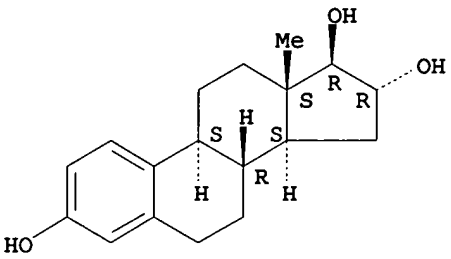
AB The present invention concerns 8β-substituted 11β-(para-substituted)phenyl estra-1,3,5(10)-trienes, e.g., I [R2 = H, I, Br, Cl, F, OH, (un)saturated O-(C1-6-alkyl) O-(C1-6-acyl), O2CPh, OCF3, OSO2NH2, OSO2NH-alkyl, OSO2N(alkyl)2, etc.; R3 = OH, OSO2NH2, OSO2NH-alkyl, OSO2N(alkyl)2, O-aryl, O-heteroaryl, O-aralkyl, etc.; R6, R7 = H; R6' = H, OH, (un)saturated O-(C1-6-alkyl) O-(C1-6-acyl), O2CPh, OCF3, OSO2NH2, OSO2NH-alkyl, OSO2N(alkyl)2, etc.; R3 = OH, OSO2NH2, OSO2NH-alkyl, OSO2N(alkyl)2, O-aryl, O-heteroaryl, O-aralkyl, etc.; R7' = H, halogen, OH, (un)saturated O-(C1-6-alkyl) O-(C1-6-acyl), O2CPh, OCF3, OSO2NH2, OSO2NH-alkyl, OSO2N(alkyl)2, etc.; R3 = OH, OSO2NH2, OSO2NH-alkyl, OSO2N(alkyl)2, O-aryl, O-heteroaryl, O-aralkyl, etc.; R8 = straight or branched-chain, optionally partly or completely halogenated C1-5-alkyl, alkenyl, ethynyl, prop-1-ynyl; R14 = H; R14R15 = bond; R15 = H; R15R16 = bond; R15' , R16' = H, halogen, OH, (un)saturated O-(C1-6-alkyl) O-(C1-6-acyl), O2CPh, OCF3, OSO2NH2, OSO2NH-alkyl, OSO2N(alkyl)2, etc.; R3 = OH, OSO2NH2, OSO2NH-alkyl, OSO2N(alkyl)2, O-aryl, O-heteroaryl, O-aralkyl, etc.; R16 = H; R17, R17' = H, H and halogen, H and O2CPh, H and OSO2OH derivative; R17R17' = :CH-halogen, O, etc.; X = O, S, bond; Y = NH2, NH(C1-10-alkyl), N(C1-10-alkyl)2, NH(C3-7-alkyl), N(C3-7-cycloalkyl)2; Z = (CH2)n; n = 1 - 12, etc.] and their pharmaceutically acceptable salts. Thus, estratrienediol II was prepared from 3-methoxyestra-1,3,5(10)-trienone III via enol trifluoromethanesulfonylation, coupling reaction with 4-PhCH2OC6H4SnBu3, hydrogenolytic debenzylation, etherification with N-(2-hydroxyethyl)piperidine, and acid-catalyzed hydrolysis. The new compds. are useful for the contraception with men and women, without affecting other **estrogenic**-sensitive organs like the uterus or the liver. They are suitable also for the treatment of benign or malicious proliferative illnesses of the ovary, like ovarian carcinomas and Granulosa cell tumors.

IT **50-27-1**, Estriol
RL: PAC (Pharmacological activity); **THU (Therapeutic use)**; BIOL (Biological study); USES (Uses)
(human **estrogen** binding ability; preparation of 8β-substituted 11β-(para-substituted)aryl-estra-2,3,5(10)-triene derivs. as contraceptives and antiproliferatives)

RN 50-27-1 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16,17-triol, (16α,17β)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



IC ICM C07J001-00
ICS A61K031-565
CC 32-3 (**Steroids**)
Section cross-reference(s): **1**, 2, **63**
ST estratriene alkyl phenyl substituted prepn contraceptive antitumor **estrogen**; proliferative illness treatment estratriene alkyl phenyl substituted; ovarian carcinoma treatment estratriene alkyl phenyl substituted; Granulosa cell tumor treatment estratriene alkyl phenyl substituted
IT **Estrogens**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 8β-substituted 11β-(para-substituted)aryl-estra-2,3,5(10)-triene derivs. as contraceptives and antiproliferatives)
IT **Estrogen** receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(α, antagonists; preparation of 8β-substituted 11β-(para-substituted)aryl-estra-2,3,5(10)-triene derivs. as contraceptives and antiproliferatives)
IT **50-27-1**, Estriol 50-28-2, Estradiol, biological studies 53-16-7, Estrone, biological studies 57-91-0, 17α-Estradiol 446-72-0, Genistein 479-13-0, Coumestrol 521-17-5, 5-Androstenediol
RL: PAC (Pharmacological activity); **THU (Therapeutic use)**; BIOL (Biological study); USES (Uses)
(human **estrogen** binding ability; preparation of 8β-substituted 11β-(para-substituted)aryl-estra-2,3,5(10)-triene derivs. as contraceptives and antiproliferatives)

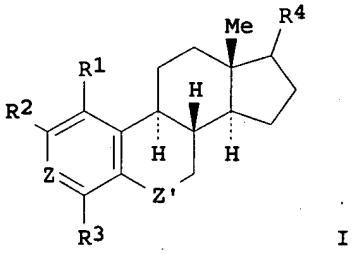
L53 ANSWER 10 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:11127 HCAPLUS
DOCUMENT NUMBER: 136:64669
TITLE: **Estrogenic** compounds as antiangiogenic agents
INVENTOR(S): D'Amato, Robert J.; Varma, Ravi K.; Haugwitz, Rudiger G.; Cushman, Mark
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 14 pp., Cont. of U.S. Ser. No. 154,322, abandoned.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

US 2002002294	A1	20020103	US 2001-899702	2001 0705
PRIORITY APPLN. INFO.:			US 1997-59916P	P 1997 0924
			US 1998-154322	B1 1998 0916

OTHER SOURCE(S): MARPAT 136:64669

GI



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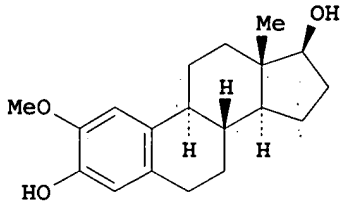


II

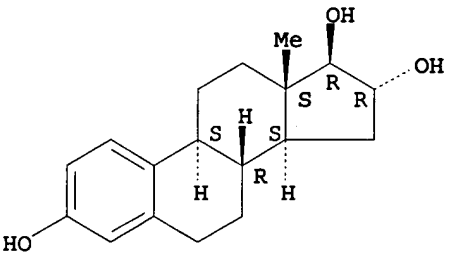
AB 2-Methoxyestradiol derivs., such as I [R1, R3 = H, Cl, Br, I, F, CN, alkyl, OH, CH2OH, NH2, alkylamino; R2 = N3, CN, C.tplbond.CR, C=CHR, RCH=CH2, C.tplbond.CH, OR, R-R1, OR-R1 (R = alkyl, R1 = OH, NH2, Cl, Br, I, F, CF3); Z = CH, COH, CR2-OH (R2 = alkyl, aralkyl); Z' = CH2, CO, CH(OH); C=NOH, C=NOR5, CHC.tplbond.N, CHNR5R5 (R5 = H, alkyl, aralkyl)], were used for treating mammalian disease characterized by undesirable angiogenesis. Thus, 2-methoxyestradiol (II) showed inhibition of tubulin polymerization (IC50 = 3.6±0.4 μM), inhibition of colchicine binding to tubulin (1.9±0.2 μM) and antitumor activity against breast, CNS, melanoma, ovarian tumor cell assay in vitro.

IT **50-27-1**, Estriol **1236-72-2**, 2-Methoxyestriol
RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); **THU (Therapeutic use)**; BIOL (Biological study); USES (Uses)
(**estrogenic** compds. as antiangiogenic agents)

RN 50-27-1 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16,17-triol, (16α,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

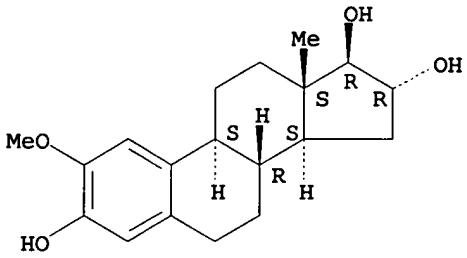


RN 1236-72-2 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16,17-triol, 2-methoxy-,

(16α,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC ICM C07J009-00
ICS C07J041-00
INCL 552009000
CC 2-4 (Mammalian Hormones)
Section cross-reference(s): **1, 32, 63**
ST **estrogen** antiangiogenic antitumor tubulin polymn inhibition; colchicine binding tubulin inhibition methoxyestradiol deriv
IT Mammary gland
(carcinoma, inhibitors; **estrogenic** compds. as antiangiogenic agents)
IT Antitumor agents
(central nervous system; **estrogenic** compds. as antiangiogenic agents)
IT Nervous system
(central, neoplasm, inhibitors; **estrogenic** compds. as antiangiogenic agents)
IT Eye
(cornea, inhibition; **estrogenic** compds. as antiangiogenic agents)
IT Angiogenesis
(**estrogenic** compds. as antiangiogenic agents)
IT Antiestrogens
Estrogens
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(**estrogenic** compds. as antiangiogenic agents)
IT Ovary, neoplasm
(inhibitors; **estrogenic** compds. as antiangiogenic agents)
IT Antitumor agents
(mammary gland carcinoma; **estrogenic** compds. as antiangiogenic agents)
IT Antitumor agents
(melanoma; **estrogenic** compds. as antiangiogenic agents)
IT Antitumor agents
(ovary; **estrogenic** compds. as antiangiogenic agents)
IT Kidney, neoplasm
(renal cell carcinoma, inhibitors; **estrogenic** compds. as antiangiogenic agents)
IT Antitumor agents
(renal cell carcinoma; **estrogenic** compds. as antiangiogenic agents)
IT Structure-activity relationship
(tubulin polymerization-inhibiting; **estrogenic** compds. as antiangiogenic agents)
IT **50-27-1**, Estriol 50-28-2, Estradiol, biological studies 53-16-7, Estrone, biological studies 56-53-1, Diethylstilbestrol 57-63-6, 17-Ethynylestradiol 64-86-8, Colchicine 362-07-2, NSC

659853 362-08-3, 2-Methoxyestrone 518-28-5, Podophyllotoxin
1035-77-4 **1236-72-2**, 2-Methoxyestriol 5976-67-0,
2-Methoxyestradiol-3-O-methyl ether 15833-07-5, 2-Bromoestradiol
16205-32-6, 2-Fluoroestradiol 22415-44-7 26788-23-8,
4-Methoxyestradiol 26890-04-0, 4-Methoxyestradiol-3-O-methyl
ether 95041-90-0 117048-59-6, Combretastatin A-4
165619-07-8, NSC 671043 165619-10-3, NSC 667049 165619-11-4,
NSC 667047 165619-22-7, NSC 673651 165619-23-8, NSC 673652
192062-02-5, NSC 682429 192062-12-7, NSC 679431 192062-13-8,
NSC 681684 192062-14-9, NSC 680185 192062-15-0, NSC 681683
192062-20-7, NSC 683125 302799-37-7, NSC 683688 383414-35-5,
NSC 678473
RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological
activity); **THU (Therapeutic use)**; BIOL (Biological
study); USES (Uses)
(**estrogenic** compds. as antiangiogenic agents)

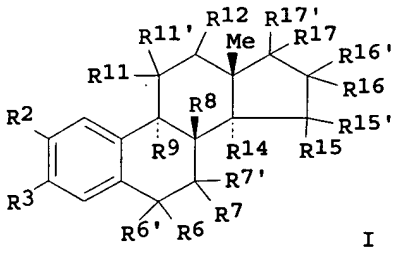
L53 ANSWER 11 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:763027 HCAPLUS
DOCUMENT NUMBER: 135:318608
TITLE: Preparation of 8β-hydrocarbyl-substituted estratrienes for use as selective **estrogens**
INVENTOR(S): Peters, Olaf; Hillisch, Alexander; Thieme, Ina; Elger, Walter; Hegele-Hartung, Christa; Kollenkirchen, Uwe; Fritzemeier, Karl-Heinrich; Patchev, Vladimir
PATENT ASSIGNEE(S): Schering Aktiengesellschaft, Germany
SOURCE: PCT Int. Appl., 90 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001077139	A1	20011018	WO 2001-EP4290	2001 0412
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
DE 10019167	A1	20011018	DE 2000-10019167	2000 0412
CA 2406177	AA	20011018	CA 2001-2406177	2001 0412
EP 1272504	A1	20030108	EP 2001-931609	2001 0412
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
BR 2001009983	A	20030225	BR 2001-9983	2001 0412
JP 2003534248	T2	20031118	JP 2001-575609	

				2001 0412
EE 200200589	A	20040415	EE 2002-589	2001 0412
ES 2245694	T3	20060116	ES 2001-1940331	2001 0412
BG 107173	A	20030530	BG 2002-107173	2002 1008
NO 2002004908	A	20021113	NO 2002-4908	2002 1011
US 2003176405	A1	20030918	US 2003-257288	2003 0401
PRIORITY APPLN. INFO.:			DE 2000-10019167 A	2000 0412
			US 2000-207370P P	2000 0526
			WO 2001-EP4290 W	2001 0412

OTHER SOURCE(S): MARPAT 135:318608

GI



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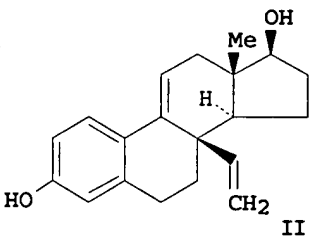
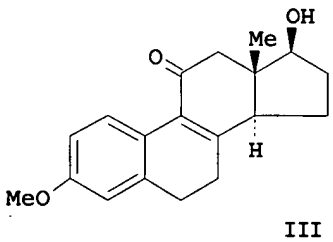


II



III

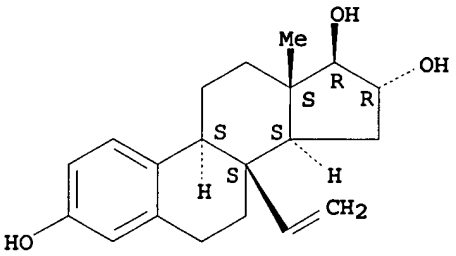
AB The invention relates to novel 8β-substituted estratrienes I [R2 = H, halogen, straight or branched (un)saturated C1-6-alkyl, alkoxy, CF3, sulfonamide; R3 = alkoxy, sulfonamide, acyloxy; R6, R7 = H; R6R7 = bond; R6', R7' = H, halogen, alkoxy, sulfonamide; R8 = a straight- or branched-chained, optionally partially or completely halogenated C1-5-alkyl, alkenyl, ethynyl, prop-1-ynyl;

R9 = H, straight or branched (un)saturated C1-5-alkyl; R9R11 = bond; R11 = H; R11R12 = bond; R11' = H, halogen, a straight- or branched-chained, optionally partially or completely fluoro- or chloro-C1-4-alkyl, alkoxy, alkylthio; R12 = H; R14 = H; R14R15 = bond; R15 = H; R15R16 = bond; R15', R16' = H, halogen, alkoxy, sulfonamid; R16 = H; R17, R17' = H, H and halogen, H and OCH2Ph, H and sulfonamide, alkyl and acyl or acyloxy, alkoxy and alkyl, alkoxy and acyloxy; R17R17' = :CH2, :CR24R25;R24, R25 = halogen; R24R25 = O]. Thus, vinylestradiol II was prepared from estra-1,3,5(10)-tetraenone III in 8 steps. The inventive estratrienes are used as pharmaceutically active substances that have in vitro a higher affinity to **estrogen** receptor prepns. of rat prostate than to **estrogen** receptor prepns. of rat uterus and which in vivo preferably have a preferential effect on bone material as compared to uterus and/or a pronounced effect with respect to the stimulation of the expression of 5HT2a receptor and transporter. II showed a relative binding affinity for the **estrogen** receptor of 1 in rat uterus and of 83 in rat prostate. The invention further relates to the production of these novel compds., to their use in therapy and to the pharmaceutical forms of administration that contain said novel compds. The invention further describes the use of said compds. for treating **estrogen**-deficiency related diseases and conditions and to the use of an 8β-substituted estratriene structural part in the overall structures of compds. that are characterized by a dissociation in favor of their **estrogen** effect on the bone as compared to the uterus.

IT **367929-22-4P 367929-25-7P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 8β-hydrocarbyl-substituted estratrienes for use as selective **estrogens**)

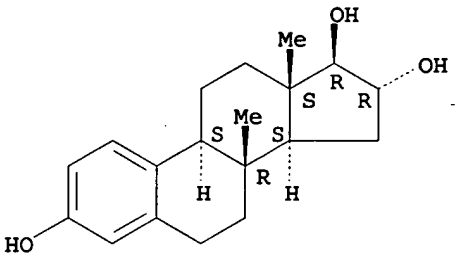
RN 367929-22-4 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16,17-triol, 8-ethenyl-, (16α,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



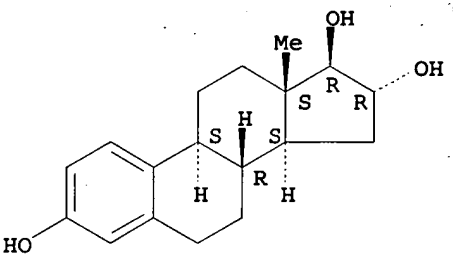
RN 367929-25-7 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16,17-triol, 8-methyl-, (16α,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **50-27-1**, Estriol
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); **THU (Therapeutic use)**; BIOL (Biological study); USES (Uses)
(preparation of 8β-hydrocarbyl-substituted estratrienes for use as selective **estrogens**)
RN 50-27-1 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16,17-triol, (16α,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC ICM C07J001-00
ICS A61K031-565; C07J041-00; A61P005-30
CC 32-3 (**Steroids**)
Section cross-reference(s): 2, **63**
ST hydrocarbyl estratriene prepn **estrogen** receptor binding; transporter 5HT2a stimulation hydrocarbyl estratriene
IT 5-HT receptors
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(5-HT2A, stimulation; preparation of 8β-hydrocarbyl-substituted estratrienes for use as selective **estrogens**)
IT **Estrogen** receptors
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(ERβ; preparation of 8β-hydrocarbyl-substituted estratrienes for use as selective **estrogens**)
IT Blood vessel, disease
Heart, disease
(circulation-related, medicaments; preparation of 8β-hydrocarbyl-substituted estratrienes for use as selective **estrogens**)
IT Nervous system
(degeneration, hormone-deficiency conditioned, medicaments; preparation of 8β-hydrocarbyl-substituted estratrienes for use as selective **estrogens**)
IT Vagina
(disease, atrophy, medicaments; preparation of 8β-hydrocarbyl-substituted estratrienes for use as selective **estrogens**
)

IT Urogenital tract
(diseases, medicaments; preparation of 8β-hydrocarbyl-substituted estratrienes for use as selective **estrogens**)
IT Fertility
Sleep
(disorder, medicaments; preparation of 8β-hydrocarbyl-substituted estratrienes for use as selective **estrogens**)
IT Bone
Prostate gland
Uterus
(**estrogen** receptor binding in; preparation of 8β-hydrocarbyl-substituted estratrienes for use as selective **estrogens**)
IT Skin
(flush, hot flashes, treatment; preparation of 8β-hydrocarbyl-substituted estratrienes for use as selective **estrogens**)
IT Blood coagulation
(hemorrhagic diathesis, medicaments; preparation of 8β-hydrocarbyl-substituted estratrienes for use as selective **estrogens**)
IT Bladder
(incontinence, medicaments; preparation of 8β-hydrocarbyl-substituted estratrienes for use as selective **estrogens**)
IT Ovary, disease
(medicament; preparation of 8β-hydrocarbyl-substituted estratrienes for use as selective **estrogens**)
IT Atherosclerosis
Hyperplasia
Intestine, disease
Osteoporosis
Stomach, disease
(medicaments; preparation of 8β-hydrocarbyl-substituted estratrienes for use as selective **estrogens**)
IT Mental disorder
(mood-affecting, medicaments; preparation of 8β-hydrocarbyl-substituted estratrienes for use as selective **estrogens**)
IT Pituitary gland, anterior lobe
(neoplasm, medicaments; preparation of 8β-hydrocarbyl-substituted estratrienes for use as selective **estrogens**)
IT Hormone replacement therapy
(preparation of 8β-hydrocarbyl-substituted estratrienes for use as selective **estrogens**)
IT **Estrogens**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 8β-hydrocarbyl-substituted estratrienes for use as selective **estrogens**)
IT Androgens
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(replacement therapy; preparation of 8β-hydrocarbyl-substituted estratrienes for use as selective **estrogens**)
IT 367929-04-2P, 3-Methoxy-8β-vinylestra-1,3,5(10)-trien-17β-ol
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)

(preparation of 8β-hydrocarbyl-substituted estratrienes for use as selective **estrogens**)

IT 26199-45-1P, 3-Methoxy-8β-methylestra-1,3,5(10)-trien-17β-ol 367264-86-6P 367264-89-9P 367929-00-8P, 3-Methoxy-8β-methylestra-1,3,5(10),9(11)-tetraen-17β-ol 367929-09-7P, 3-Methoxy-8β-vinyl-1,3,5(10)-trien-17α-ol 367929-14-4P, 3-Methoxy-17α-(trifluoromethyl)-8β-vinylestra-1,3,5(10)-trien-17β-ol
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of 8β-hydrocarbyl-substituted estratrienes for use as selective **estrogens**)

IT 3327-97-7P, 8β-Methylestra-1,3,5(10)-triene-3,17β-diol 367264-78-6P 367264-79-7P 367264-81-1P 367264-83-3P 367264-85-5P 367264-87-7P 367264-90-2P 367264-92-4P 367264-95-7P 367929-01-9P, 8β-Vinylestra-1,3,5(10),9(11)-tetraene-3,17β-ol 367929-02-0P 367929-03-1P 367929-07-5P, 8β-Methylestra-1,3,5(10),9(11)-tetraene-3,17β-diol 367929-08-6P, 8β-Ethyl-9β-estra-1,3,5(10)-triene-3,17β-ol 367929-10-0P, 8β-Vinyl-1,3,5(10)-triene-3,17α-diol 367929-11-1P, 17α-Trifluoromethyl-8β-vinylestra-1,3,5(10)-triene-3,17β-diol 367929-12-2P, 8β-Vinylestra-1,3,5(10)-triene-2,3,17β-triol 367929-15-5P 367929-16-6P 367929-17-7P 367929-18-8P 367929-19-9P 367929-20-2P 367929-21-3P **367929-22-4P** 367929-23-5P 367929-24-6P **367929-25-7P** 367929-26-8P 367929-27-9P 367929-28-0P 367929-29-1P 367929-30-4P 367929-31-5P 367929-32-6P 367929-33-7P 367929-34-8P, 8β-Vinyl-9β-estra-1,3,5(10)-triene-3,17β-diol
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 8β-hydrocarbyl-substituted estratrienes for use as selective **estrogens**)

IT **50-27-1**, Estriol 50-28-2, Estradiol, biological studies 53-16-7, Estrone, biological studies 57-91-0, 17α-Estradiol 446-72-0, Genistein 479-13-0, Coumestrol 521-17-5, 5-Androstenediol
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); **THU (Therapeutic use)**; BIOL (Biological study); USES (Uses)
(preparation of 8β-hydrocarbyl-substituted estratrienes for use as selective **estrogens**)

IT 1478-53-1, Diethyl (difluoromethyl)phosphonate 17401-32-0 367929-13-3, 3,17β-Bis[(tetrahydropyran-2-yl)oxy]-8β-vinylestra-1,3,5(10)-triene
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of 8β-hydrocarbyl-substituted estratrienes for use as selective **estrogens**)

IT 28990-61-6P, 8β-Formyl-3-methoxyestra-1,3,5(10),9(11)-tetraen-17β-ol 367264-68-4P 367264-69-5P 367264-70-8P 367264-71-9P 367264-72-0P 367264-73-1P 367264-74-2P 367264-75-3P 367264-76-4P 367264-77-5P 367264-80-0P 367264-82-2P 367264-84-4P 367264-88-8P 367264-91-3P 367264-93-5P 367264-94-6P 367264-96-8P 367279-41-2P 367929-05-3P, 3-Methoxy-8β-vinylestra-1,3,5(10)-trien-17-one 367929-06-4P, 3-Hydroxy-8β-vinylestra-1,3,5(10)-trien-17-one
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 8β-hydrocarbyl-substituted estratrienes for use as selective **estrogens**)

REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE

FOR THIS RECORD. ALL CITATIONS AVAILABLE
IN THE RE FORMAT

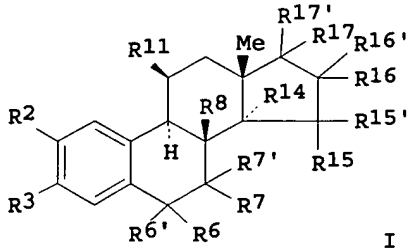
L53 ANSWER 12 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:763026 HCAPLUS
DOCUMENT NUMBER: 135:318607
TITLE: Preparation of 8β-substituted-11β-pentyl- and 11β-hexyl-estra-1,3,5(10)-triene derivatives which have an affinity for the **estrogen** receptor
INVENTOR(S): Peters, Olaf; Braeuer, Nico; Hillisch, Alexander; Hegele-Hartung, Christa; Fritzemeier, Karl-Heinrich
PATENT ASSIGNEE(S): Schering Aktiengesellschaft, Germany
SOURCE: PCT Int. Appl., 53 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001077138	A1	20011018	WO 2001-EP4289	2001 0412
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CO, CR, CU, CZ, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
DE 10019167	A1	20011018	DE 2000-10019167	2000 0412
EP 1272505	A1	20030108	EP 2001-940331	2001 0412
EP 1272505	B1	20050824		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2003530403	T2	20031014	JP 2001-575608	2001 0412
AT 302790	E	20050915	AT 2001-940331	2001 0412
ES 2245694	T3	20060116	ES 2001-1940331	2001 0412
NO 2002004907	A	20021205	NO 2002-4907	2002 1011
US 2004029847	A1	20040212	US 2003-257287	2003 0708
PRIORITY APPLN. INFO.:			DE 2000-10019167 A	2000 0412
			US 2000-207370P P	

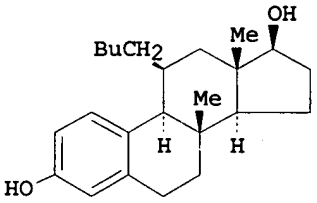
2000
0526

WO 2001-EP4289 W
2001
0412

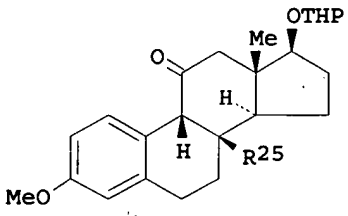
OTHER SOURCE(S): MARPAT 135:318607
GI



I



II



III

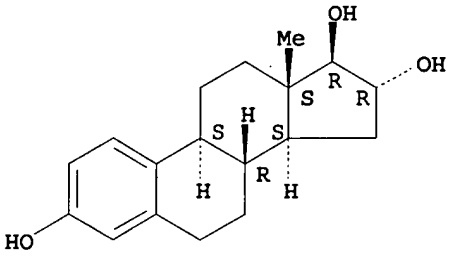
AB The present invention relates to the novel 8β-substituted estra-1,3,5(10)-trienes I [R2 = H, F, Cl, Br, I, straight or branched (un)saturated C1-6-alkyl, OH, alkoxy, acyloxy, CF3, sulfamoyloxy; R3 = alkoxy, sulfamoyloxy, acyloxy; R6, R6' = H; R6R7 = bond; R7, R7' = H ; R8 means a straight-chain or branched-chain, optionally partially or entirely halogenated alkyl or alkenyl radical having up to 5 carbon atoms, an ethynyl or prop-1-inyl radical; R11 = pentyl, hexyl; R14 = H; R14R15 = bond ; R15 = H; R15', R16' = H, F, Cl, Br, I, alkoxy, sulfamoyloxy, acyloxy; R15R16 = bond; R16 = H; R17, R17' = H, H and halogen, H and OCH2Ph, H and sulfamoyloxy; alkyl and acyl or acyloxy; alkoxy and alkyl, alkoxy and acyloxy; R17R17' = CH2 CR23R24; R23, R24 = H, halogen; R23R24 = O]. Thus, 8β-methyl-11β-pentyl-1,3,5(10)-triene-3,17β-diol (II) was prepared from 8β-cyanosteroid III (R25 = CN) via condensation of 11-ketosteroid III (R25 = Me) with BuCH2Li. Estradienes I are used as pharmaceutical active agents which, in vitro, are provided with a higher affinity of **estrogen** receptor prepns. of rat prostate than of **estrogen** receptor prepns. of rat uterus and, in vivo, preferably act in a preferential contraceptive manner on the ovary without stimulating the uterus. The invention also relates to the production thereof, the therapeutic use thereof and pharmaceutical administration forms which contain the novel compds. I. The invention further relates to the use of compds. I for male contraception and to the use of non-malignant or malignant proliferate diseases of the ovary, such as ovarian carcinoma or granulosa cell tumors for instance.

IT **50-27-1**, Estriol
RL: BAC (Biological activity or effector, except adverse); BSU

(Biological study, unclassified); **THU (Therapeutic use)**; BIOL (Biological study); USES (Uses)
(preparation of 8β-substituted-11β-pentyl- and -11β-hexyl-estra-1,3,5(10)-triene derivs. which have an affinity for the **estrogen** receptor)

RN 50-27-1 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16,17-triol, (16α,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC ICM C07J001-00
ICS A61K031-565; C07J041-00; A61P005-30
CC 32-3 (**Steroids**)
Section cross-reference(s): **1**, 2, **63**
ST estratriene pentyl hexyl deriv prepn **estrogen** receptor binding affinity; contraceptive estratriene pentyl hexyl deriv prepn; ovarian proliferate disease inhibitor estratriene pentyl hexyl deriv prepn; granulosa cell tumor inhibitor estratriene pentyl hexyl deriv prepn
IT Hormone replacement therapy
(GnHR antagonists; preparation of 8β-substituted-11β-pentyl- and -11β-hexyl-estra-1,3,5(10)-triene derivs. which have an affinity for the **estrogen** receptor)
IT Progesterone receptors
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(antagonists; preparation of 8β-substituted-11β-pentyl- and -11β-hexyl-estra-1,3,5(10)-triene derivs. which have an affinity for the **estrogen** receptor)
IT Ovary, neoplasm
(carcinoma, inhibitors; preparation of 8β-substituted-11β-pentyl- and -11β-hexyl-estra-1,3,5(10)-triene derivs. which have an affinity for the **estrogen** receptor)
IT Ovary
(contraceptives affecting; preparation of 8β-substituted-11β-pentyl- and -11β-hexyl-estra-1,3,5(10)-triene derivs. which have an affinity for the **estrogen** receptor)
IT Prostate gland
Uterus
(**estrogen** receptor affinity; preparation of 8β-substituted-11β-pentyl- and -11β-hexyl-estra-1,3,5(10)-triene derivs. which have an affinity for the **estrogen** receptor)
IT Contraceptives
(female; preparation of 8β-substituted-11β-pentyl- and -11β-hexyl-estra-1,3,5(10)-triene derivs. which have an affinity for the **estrogen** receptor)
IT Progestogens
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(gestagens and mesoprogestins; preparation of 8β-substituted-11β-pentyl- and -11β-hexyl-estra-1,3,5(10)-triene derivs. which have an affinity for the **estrogen** receptor)

IT Ovary, neoplasm
(granulosa cell tumor, inhibitors; preparation of 8β-substituted-11β-pentyl- and -11β-hexyl-estra-1,3,5(10)-triene derivs. which have an affinity for the **estrogen** receptor)

IT Antitumor agents
(granulosa cell tumor; preparation of 8β-substituted-11β-pentyl- and -11β-hexyl-estra-1,3,5(10)-triene derivs. which have an affinity for the **estrogen** receptor)

IT Contraceptives
(male; preparation of 8β-substituted-11β-pentyl- and -11β-hexyl-estra-1,3,5(10)-triene derivs. which have an affinity for the **estrogen** receptor)

IT Antitumor agents
(ovary carcinoma; preparation of 8β-substituted-11β-pentyl- and -11β-hexyl-estra-1,3,5(10)-triene derivs. which have an affinity for the **estrogen** receptor)

IT **Estrogens**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of 8β-substituted-11β-pentyl- and -11β-hexyl-estra-1,3,5(10)-triene derivs. which have an affinity for the **estrogen** receptor)

IT **Estrogen** receptors
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(preparation of 8β-substituted-11β-pentyl- and -11β-hexyl-estra-1,3,5(10)-triene derivs. which have an affinity for the **estrogen** receptor)

IT Disease, animal
(proliferative, ovarian, inhibitors; preparation of 8β-substituted-11β-pentyl- and -11β-hexyl-estra-1,3,5(10)-triene derivs. which have an affinity for the **estrogen** receptor)

IT 367269-62-3P, 3-Methoxy-8β-methyl-11-pentylestra-1,3,5(10),9(11)-tetraen-17β-ol 367269-63-4P, 11-Hexyl-3-methoxy-8β-methylestra-1,3,5(10),9(11)-tetraen-17β-ol 367269-64-5P, 3-Methoxy-8β-methyl-11β-pentylestra-1,3,5(10)-trien-17β-ol 367269-65-6P, 11β-Hexyl-3-methoxy-8β-methylestra-1,3,5(10)-trien-17β-ol 367269-77-0P, 3-Methoxy-11β-pentyl-8β-vinylestra-1,3,5(10)-trien-17β-ol 367269-78-1P, 11β-Hexyl-3-methoxy-8β-vinylestra-1,3,5(10)-trien-17β-ol
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of 8β-substituted-11β-pentyl- and -11β-hexyl-estra-1,3,5(10)-triene derivs. which have an affinity for the **estrogen** receptor)

IT 367269-66-7P, 8β-Methyl-11β-pentylestra-1,3,5(10)-triene-3,17β-diol 367269-67-8P, 11β-Hexyl-8β-methylestra-1,3,5(10)-triene-3,17β-diol 367269-79-2P, 11β-Pentyl-8β-vinylestra-1,3,5(10)-triene-3,17β-diol 367269-80-5P, 11β-Hexyl-8β-vinylestra-1,3,5(10)-triene-3,17β-diol 367269-81-6P, 8β-Ethyl-11β-pentyl-1,3,5(10)-triene-3,17β-diol 367269-82-7P, 8β-Ethyl-11β-hexyl-1,3,5(10)-triene-3,17β-diol 367269-83-8P, 8β-Methyl-11β-pentyl-1,3,5(10)-triene-

3,17β-diol 3-sulfamate 367269-84-9P, 8β-Ethyl-11β-pentyl-1,3,5(10)-triene-3,17β-diol 3-sulfamate 367269-85-0P, 11β-Pentyl-8β-vinyl-1,3,5(10)-triene-3,17β-diol 3-sulfamate 367269-86-1P, 11β-Hexyl-8β-methyl-1,3,5(10)-triene-3,17β-diol 3-sulfamate 367269-87-2P, 8β-Ethyl-11β-hexyl-1,3,5(10)-triene-3,17β-diol 3-sulfamate 367269-88-3P, 11β-Hexyl-8β-vinyl-1,3,5(10)-triene-3,17β-diol 3-sulfamate 367269-89-4P, 8β-Methyl-11β-pentyl-1,3,5(10)-triene-3,17β-diol 3-acetate 367269-90-7P, 8β-Ethyl-11β-pentyl-1,3,5(10)-triene-3,17β-diol 3-acetate 367269-91-8P, 11β-Pentyl-8β-vinyl-1,3,5(10)-triene-3,17β-diol 3-acetate 367269-92-9P, 11β-Hexyl-8β-methyl-1,3,5(10)-triene-3,17β-diol 3-acetate 367269-93-0P, 8β-Ethyl-11β-hexyl-1,3,5(10)-triene-3,17β-diol 3-acetate 367269-94-1P, 11β-Hexyl-8β-vinyl-1,3,5(10)-triene-3,17β-diol 3-acetate
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 8β-substituted-11β-pentyl- and -11β-hexyl-estra-1,3,5(10)-triene derivs. which have an affinity for the **estrogen** receptor)

IT **50-27-1**, Estriol 50-28-2, Estradiol, biological studies 53-16-7, Estrone, biological studies 57-91-0, 17α-Estradiol 446-72-0, Genistein 479-13-0, Coumestrol 521-17-5, 5-Androstenediol
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); **THU (Therapeutic use)**; BIOL (Biological study); USES (Uses)
(preparation of 8β-substituted-11β-pentyl- and -11β-hexyl-estra-1,3,5(10)-triene derivs. which have an affinity for the **estrogen** receptor)

IT 3525-31-3, Pentyllithium 21369-64-2, Hexyllithium 367269-56-5 367269-68-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of 8β-substituted-11β-pentyl- and -11β-hexyl-estra-1,3,5(10)-triene derivs. which have an affinity for the **estrogen** receptor)

IT 367269-57-6P 367269-58-7P 367269-59-8P 367269-60-1P 367269-61-2P 367269-69-0P 367269-70-3P 367269-71-4P, 8β-Cyano-3-methoxy-11β-pentylestra-1,3,5(10,9(11)-tetraen-17β-ol 367269-72-5P, 8β-Cyano-11β-hexyl-3-methoxyestra-1,3,5(10,9(11)-tetraen-17β-ol 367269-73-6P, 8β-Formyl-3-methoxy-11β-pentylestra-1,3,5(10),9(11)-tetraen-17β-ol 367269-74-7P, 8β-Formyl-11β-hexyl-3-methoxyestra-1,3,5(10),9(11)-tetraen-17β-ol 367269-75-8P, 8β-Formyl-3-methoxy-11β-pentylestra-1,3,5(10)-trien-17β-ol 367269-76-9P, 8β-Formyl-11β-hexyl-3-methoxyestra-1,3,5(10)-trien-17β-ol
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 8β-substituted-11β-pentyl- and -11β-hexyl-estra-1,3,5(10)-triene derivs. which have an affinity for the **estrogen** receptor)

REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L53 ANSWER 13 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1997:192107 HCAPLUS
DOCUMENT NUMBER: 126:190942
TITLE: Transdermal administration of esters of 13-ethyl-17β-hydroxy-11-methylene-18,19-dinor-17-α-pregn-4-en-20-yn-3-one

INVENTOR(S): Lipp, Ralph; Ewers, Christian L. J.; Guenther, Clemens; Riedl, Jutta; Taeuber, Ulrich
PATENT ASSIGNEE(S): Schering A.-G., Germany
SOURCE: Ger. Offen., 11 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19613698	A1	19970123	DE 1996-19613698	1996 0401
WO 9703709	A1	19970206	WO 1996-EP3033	1996 0706
W: AU, BR, CA, CN, CZ, FI, HU, IL, JP, KR, MX, NO, NZ, PL, RU, SK, UA, US, VN				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
AU 9666140	A1	19970218	AU 1996-66140	1996 0706
EP 848620	A1	19980624	EP 1996-925717	1996 0706
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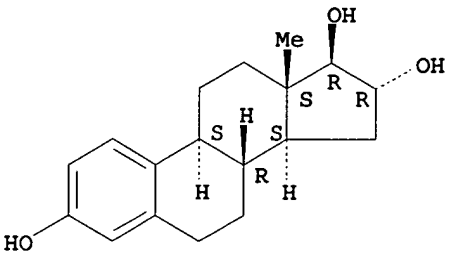
JP 11509222	T2	19990817	JP 1996-506250	1996 0706
ZA 9606083	A	19980619	ZA 1996-6083	1996 0717
PRIORITY APPLN. INFO.:			DE 1995-19526789 A1	1995 0717
			DE 1996-19613698 A	1996 0401
			WO 1996-EP3033 W	1996 0706

AB The title compds. in combination with 1 or more **estrogens** are suitable for the transdermal administration and therapy of diseases such as osteoporosis. Thus, 0.8 g 13-ethyl-17β-hexanoyloxy-11-methylene-18,19-dinor-17-α-pregn-4-en-20-yn-3-one (preparation method given) and 8.0 g dimethylisosorbide were mixed in 62.4 g 50% solution of silicone rubber in petrol. This mixture was coated on a polyester film and the laminate could be used for transdermal hormone delivery.

IT **50-27-1**, Estriol **187538-69-8**
RL: **THU (Therapeutic use)**; BIOL (Biological study); USES (Uses)
(transdermal administration of dinorpregnynone esters)

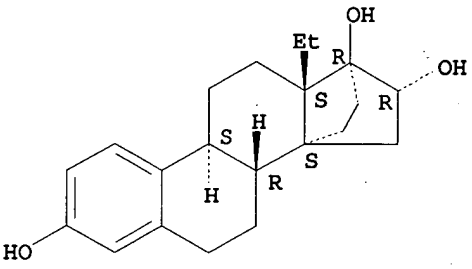
RN 50-27-1 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16,17-triol, (16α,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 187538-69-8 HCAPLUS
CN 14,21-Cyclo-18,19-dinorpregna-1,3,5(10)-triene-3,16,17-triol, 13-ethyl-, (16α,17α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC ICM C07J001-00
ICS A61K031-565; A61L015-44
CC 63-6 (**Pharmaceuticals**)
Section cross-reference(s): 2, **32**
ST dinorpregnynone ester **estrogen** transdermal prepn
IT **Estrogens**
Osteoporosis
Ovarian cycle
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(transdermal administration of dinorpregnynone esters)
IT **50-27-1**, Estriol 50-28-2, Estradiol, biological studies
57-63-6, 17α-EthinylEstradiol 72-33-3, Mestranol
54048-10-1 54048-10-1D, esters 187538-68-7 **187538-69-8**
RL: **THU (Therapeutic use)**; BIOL (Biological study); USES (Uses)
(transdermal administration of dinorpregnynone esters)

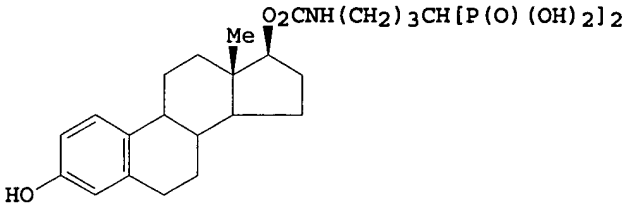
L53 ANSWER 14 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1992:612787 HCAPLUS
DOCUMENT NUMBER: 117:212787
TITLE: Preparation and formulation of [bis(phosphono)butylaminocarbonyloxy]estratriene and analogs for treatment of bone disease
INVENTOR(S): Saari, Walfred S.; Rodan, Gideon A.; Fisher, Thorsten E.; Anderson, Paul S.
PATENT ASSIGNEE(S): Merck and Co., Inc., USA
SOURCE: Eur. Pat. Appl., 21 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

EP 496520	A1	19920729	EP 1992-300291	1992 0114
R: CH, DE, FR, GB, IT, LI, NL				
CA 2059421	AA	19920723	CA 1992-2059421	1992 0115
JP 04352795	A2	19921207	JP 1992-8786	1992 0122
JP 07035395	B4	19950419		
US 5183815	A	19930202	US 1992-839741	1992 0219
PRIORITY APPLN. INFO.:			US 1991-644178 A	1991 0122

OTHER SOURCE(S): MARPAT 117:212787

GI



II

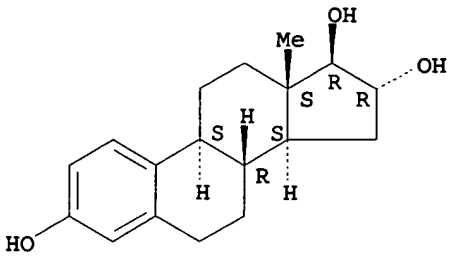
AB Compds. ABC [A = residue of a hydroxy-containing steroidal hormone having human bone resorption-antagonist activity or bone formation-stimulatory activity; C = residue of an amino- or hydroxyalkyl-1,1-bis(phosphonate) having human bone affinity; B = covalent linkage connecting A through the hydroxyl moiety and C through the amino or hydroxyl moiety, which linkage can hydrolyze in the human body in the vicinity of bone to release steroidal hormone A] were prepared for treatment of bone disorders (no data). Thus, [(Me2CHO)2P(O)]2CHR (I; R = H), was condensed with CH2:CHCN and the product hydrogenated to give I [R = (CH2)3NH2], which was condensed with 3-benzyloxy-17β-chlorocarbonyloxyestra-1,3,5(10)-triene (preparation given) to give, after deprotection, title compound II.

IT **50-27-1DP**, derivs. linked to bisphosphonate moieties
RL: **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, for treatment of bone disease)

RN 50-27-1 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16,17-triol, (16α,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC ICM C07J051-00
ICS A61K031-565; C07F009-40
CC 32-3 (**Steroids**)
Section cross-reference(s): **1**, 29, **63**
IT 50-02-2DP, derivs. linked to bisphosphonate moieties 50-03-3DP, derivs. linked to bisphosphonate moieties 50-22-6DP, derivs. linked to bisphosphonate moieties 50-23-7DP, derivs. linked to bisphosphonate moieties 50-24-8DP, derivs. linked to bisphosphonate moieties **50-27-1DP**, derivs. linked to bisphosphonate moieties 50-28-2DP, Estra-1,3,5(10)-triene-3,17-diol (17β)-, derivs. linked to bisphosphonate moieties 50-50-0DP, derivs. linked to bisphosphonate moieties 52-76-6DP, derivs. linked to bisphosphonate moieties 52-78-8DP, derivs. linked to bisphosphonate moieties 53-03-2DP, derivs. linked to bisphosphonate moieties 53-06-5DP, derivs. linked to bisphosphonate moieties 53-33-8DP, derivs. linked to bisphosphonate moieties 53-34-9DP, derivs. linked to bisphosphonate moieties 53-39-4DP, derivs. linked to bisphosphonate moieties 53-41-8DP, derivs. linked to bisphosphonate moieties 53-43-0DP, derivs. linked to bisphosphonate moieties 57-63-6DP, derivs. linked to bisphosphonate moieties 58-18-4DP, derivs. linked to bisphosphonate moieties 58-22-0DP, derivs. linked to bisphosphonate moieties 67-73-2DP, derivs. linked to bisphosphonate moieties 67-81-2DP, derivs. linked to bisphosphonate moieties 68-22-4DP, derivs. linked to bisphosphonate moieties 68-23-5DP, derivs. linked to bisphosphonate moieties 68-96-2DP, derivs. linked to bisphosphonate moieties 72-33-3DP, derivs. linked to bisphosphonate moieties 72-63-9DP, derivs. linked to bisphosphonate moieties 76-25-5DP, derivs. linked to bisphosphonate moieties 76-43-7DP, derivs. linked to bisphosphonate moieties 76-47-1DP, derivs. linked to bisphosphonate moieties 79-64-1DP, derivs. linked to bisphosphonate moieties 83-43-2DP, derivs. linked to bisphosphonate moieties 124-94-7DP, derivs. linked to bisphosphonate moieties 125-02-0DP, derivs. linked to bisphosphonate moieties 125-04-2DP, derivs. linked to bisphosphonate moieties 145-12-0DP, derivs. linked to bisphosphonate moieties 152-43-2DP, derivs. linked to bisphosphonate moieties 152-97-6DP, derivs. linked to bisphosphonate moieties 153-00-4DP, derivs. linked to bisphosphonate moieties 356-12-7DP, derivs. linked to bisphosphonate moieties 360-66-7DP, derivs. linked to bisphosphonate moieties 378-44-9DP, derivs. linked to bisphosphonate moieties 382-67-2DP, derivs. linked to bisphosphonate moieties 426-13-1DP, derivs. linked to bisphosphonate moieties 432-60-0DP, derivs. linked to bisphosphonate moieties 434-03-7DP, derivs. linked to bisphosphonate moieties 434-07-1DP, derivs. linked to bisphosphonate moieties 434-22-0DP, derivs. linked to bisphosphonate moieties 471-53-4DP, derivs. linked to bisphosphonate moieties 474-86-2DP, derivs. linked to

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bisphosphonate moieties
RL: **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, for treatment of bone disease)

L53 ANSWER 15 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1987:5325 HCAPLUS
DOCUMENT NUMBER: 106:5325
TITLE: Estradiol and estriol glycolates
INVENTOR(S): Duesterberg, Bernd; Acksteiner, Bernard; Schulze, Paul Eberhard
PATENT ASSIGNEE(S): Schering A.-G., Fed. Rep. Ger.
SOURCE: Ger. Offen., 12 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3511587	A1	19861002	DE 1985-3511587	19850327
EP 196271	A2	19861001	EP 1986-730052	19860320
EP 196271	A3	19870204		
EP 196271	B1	19890208		
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
AT 40695	E	19890215	AT 1986-730052	19860320
JP 61221198	A2	19861001	JP 1986-67418	19860327
US 4780460	A	19881025	US 1986-845102	19860327

PRIORITY APPLN. INFO.: DE 1985-3511587 A 19850327
EP 1986-730052 A 19860320

OTHER SOURCE(S): CASREACT 106:5325; MARPAT 106:5325

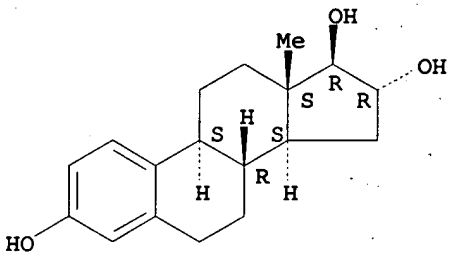
AB Title esters RO2CCH2Z (R = residue of estradiol or estriol; Z = OH, O2CR1; R1 = Me, Ph) are prepared as **estrogens** (no data), usable as aqueous crystalline suspensions in long-acting injectable contraceptives. Thus, esterification of estradiol with PhCO2CH2COCl in C2Cl4 in the presence of collidine gave estradiol 3,17β-bis(benzoyloxyacetate), which was saponified to give estradiol 17β-benzoyloxyacetate (I). An injectable 1-mL saline suspension containing microcryst. I and norethisterone 17β-benzoyloxyacetate was prepared as a 1-mo contraceptive.

IT **50-27-1**, Estriol
RL: RCT (Reactant); RACT (Reactant or reagent)
(esterification of, with acetoxyacetyl and benzoyloxyacetyl chlorides)

RN 50-27-1 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16,17-triol, (16α,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC ICM C07J001-00
ICS A61K031-565

CC 32-3 (**Steroids**)
Section cross-reference(s): 2, **63**

ST glycolate estradiol estriol prepn **estrogen**; contraceptive estradiol estriol glycolate prepn; injection contraceptive estradiol estriol glycolate

IT **Estrogens**
RL: RCT (Reactant); RACT (Reactant or reagent)
(estradiol and estriol glycolates)

IT **50-27-1**, Estriol 50-28-2, Estradiol, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(esterification of, with acetoxyacetyl and benzoyloxyacetyl chlorides)

IT 105426-11-7P, Estradiol 17β-benzoyloxyacetate 105579-76-8P, Estradiol 3,17β-bis(acetoxyacetate) 105579-77-9P, Estradiol 17β-acetoxyacetate 105579-78-0P, Estradiol 17β-glycolate 105579-79-1P 105579-80-4P, Estriol 3,16α,17β-tris(acetoxyacetate) 105579-81-5P, Estriol 16α,17β-bis(acetoxyacetate) 105579-82-6P 105579-83-7P, Estriol 16α,17β-bis(benzoyloxyacetate)
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as **estrogen**)

L53 ANSWER 16 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1975:175239 HCAPLUS
DOCUMENT NUMBER: 82:175239
TITLE: 17α-Ethynylestriol-3-cyclopentyl ether
INVENTOR(S): Kraay, Russell J.; Farkas, Eugene
PATENT ASSIGNEE(S): Eli Lilly and Co., USA
SOURCE: U.S., 7 pp. Division of U.S. 3,790,605 (CA 80;121211e).
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 5
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3868452	A	19750225	US 1973-411988	1973 1101
US 3790605	A	19740205	US 1971-136671	1971 0423
PRIORITY APPLN. INFO.:			US 1971-127690 A2	1971 0324
			US 1971-136671 A3	1971 0423

GI For diagram(s), see printed CA Issue.

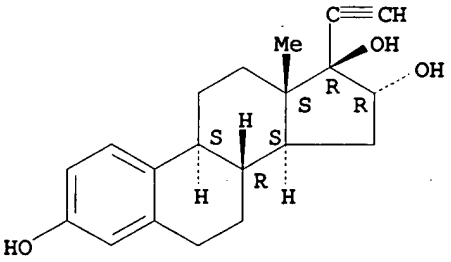
AB 17α-Ethynylestriol 3-cyclopentyl ether (I) [39791-20-3], a potent **estrogen** was useful in doses of 5-500 μg/day in treatment of menopausal syndrome and other conditions of **estrogen** deficiency or in which **estrogens** may be used therapeutically. 16α-Hydroxyestrone diacetate [1247-71-8] treated with ethynylmagnesium bromide gave 17α-ethynylestriol [**4717-40-2**] and the 17β-isomer [**10098-79-0**]. Elution with MeOH, washing with CHCl3 and recrsytn. from EtOAc-hexane mixture gave pure α-isomer, which was converted to Na salt [**53154-93-1**]. Treatment with cyclopentyl bromide [137-43-9] in formamide solution gave I, recrystd. from ether-hexane mixture, m. about 162-5°. Pharmacol. tests and pharmaceutical formulations were given.

IT **53154-93-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with cyclopentyl bromide)

RN 53154-93-1 HCAPLUS

CN 19-Norpregna-1,3,5(10)-trien-20-yne-3,16,17-triol, monosodium salt, (16α,17α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● Na

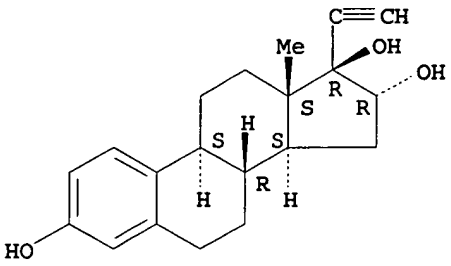
IT **4717-40-2P**
RL: PREP (Preparation)
(preparation and sodium salt formation of)

RN 4717-40-2 HCAPLUS

CN 19-Norpregna-1,3,5(10)-trien-20-yne-3,16,17-triol,

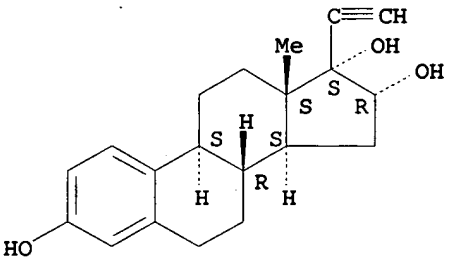
(16α,17α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **10098-79-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 10098-79-0 HCAPLUS
CN 19-Norpregna-1,3,5(10)-trien-20-yne-3,16,17-triol, (16α)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC A61K
INCL 424238000
CC 63-6 (**Pharmaceuticals**)
Section cross-reference(s): **2, 32**
IT **53154-93-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP
(Preparation); RACT (Reactant or reagent)
(preparation and reaction with cyclopentyl bromide)
IT **4717-40-2P**
RL: PREP (Preparation)
(preparation and sodium salt formation of)
IT **10098-79-0P** 39791-18-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

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L12 289 SEA FILE=REGISTRY ABB=ON PLU=ON (10449-00-0/BI OR
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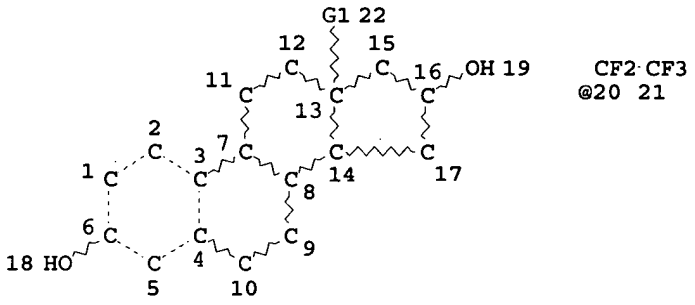
L13 SCR 1844
L14 STR



VAR G1=ME/ET/CF3/20
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 22

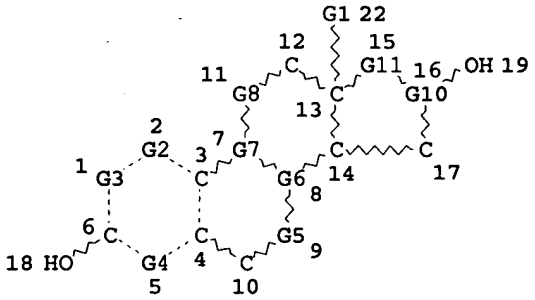
STEREO ATTRIBUTES: NONE
L15 899 SEA FILE=REGISTRY SSS FUL L14 NOT L13
L16 266 SEA FILE=REGISTRY ABB=ON PLU=ON L12 AND L15
L25 STR

CF2·CF3 @20 21 | C~X @23 24 | C~CF3 @25 26 | C~OH @27 28 | C~Me @29 30 | C~OMe @31 32

C~OEt @33 34 | C~Ak @35 36 | C~O~Ak @37 38 39 | C~CF2·CF3 @42 41 40 | C~Ak~F @43 44 45

C~Cy @46 47 | C~CN @48 49 | C~Et @50 51 | C~O~NO2 @52 53 54 | C~CH2Cl @55 56 57

C~G9 @58 59 | C~S~Ak @60 61 63 | S @62



C~CH2·CN @64 65 66 | C~F @67 68

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VAR G3=CH/23/27/35/37
VAR G4=CH/23/35/25/42/37
VAR G5=CH/23/35/43/37/46
VAR G6=CH/35/43/48
VAR G7=CH/29/50/25/42
VAR G8=CH2/CH/52/27/58/23/55/35/43/37/46
VAR G9=62/60
VAR G10=CH/35/43/25/42/64
VAR G11=CH2/CH/67/35/43
NODE ATTRIBUTES:
CONNECT IS E2 RC AT 61
CONNECT IS E1 RC AT 62
DEFAULT MLEVEL IS ATOM
GGCAT IS UNS AT 47
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 68

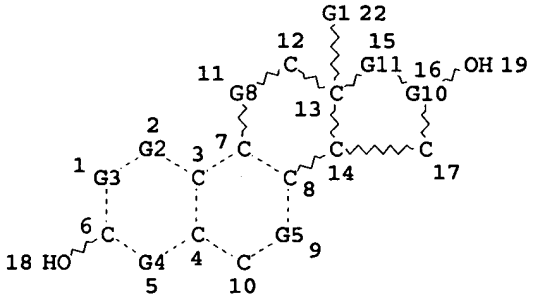
STEREO ATTRIBUTES: NONE
L26 STR

CF2·CF3 C~X C~CF3 C~OH C~Me C~OMe
@20 21 @23 24 @25 26 @27 28 @29 30 @31 32

C~OEt C~Ak C~O~Ak C~CF2·CF3 C~Ak~F
@33 34 @35 36 @37 38 39 @42 41 40 @43 44 45

C~Cy C~CN C~Et C~O~NO2 C~CH2Cl
@46 47 48 49 50 51 @52 53 54 @55 56 57

C~G9 C~S~Ak S @62
@58 59 @60 61 63



C~CH2·CN C~F
@64 65 66 @67 68

VAR G1=ME/ET/CF3/20
VAR G2=CH/23/27/25/29/31/33
VAR G3=CH/23/27/35/37
VAR G4=CH/23/35/25/42/37
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VAR G9=62/60
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VAR G11=CH2/CH/67/35/43
NODE ATTRIBUTES:
CONNECT IS E2 RC AT 61
CONNECT IS E1 RC AT 62
DEFAULT MLEVEL IS ATOM
GGCAT IS UNS AT 47
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 68

STEREO ATTRIBUTES: NONE

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L34	46181	SEA FILE=HCAPLUS ABB=ON PLU=ON	STEROID?/SC,SX
L35	362	SEA FILE=HCAPLUS ABB=ON PLU=ON	L31 AND L34
L36	316	SEA FILE=HCAPLUS ABB=ON PLU=ON	L32 AND L34
L37	2051502	SEA FILE=HCAPLUS ABB=ON PLU=ON	PHARMA?/SC,SX
L38	1679	SEA FILE=HCAPLUS ABB=ON PLU=ON	L37 AND L31
L39	652504	SEA FILE=HCAPLUS ABB=ON PLU=ON	PHARMACEU?/SC,SX
L40	410	SEA FILE=HCAPLUS ABB=ON PLU=ON	L39 AND L31
L41	404	SEA FILE=HCAPLUS ABB=ON PLU=ON	L39 AND L32
L42	27	SEA FILE=HCAPLUS ABB=ON PLU=ON	L35 AND L36 AND L38 AND L40 AND L41
L43	50	SEA FILE=HCAPLUS ABB=ON PLU=ON	L42 OR L33

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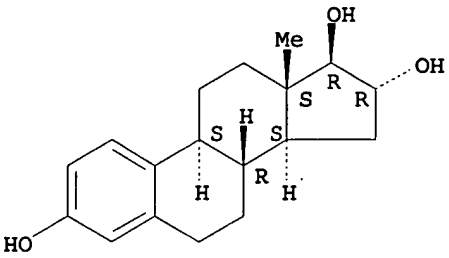
L56            9 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L55 AND L54


=> d l56 1-9 ibib abs hitstr hitind

L56  ANSWER 1 OF 9  HCAPLUS  COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER:         1999:607548  HCAPLUS
DOCUMENT NUMBER:          131:337760
TITLE:                    Solubilization of hydrophobic compounds by
                          micellar solutions of hydrophobically modified
                          polyelectrolytes
AUTHOR(S):                Bromberg, Lev; Temchenko, Marina
CORPORATE SOURCE:         Department of Materials Science and
                          Engineering, Massachusetts Institute of
                          Technology, Cambridge, MA, 02139, USA
SOURCE:                   Langmuir (1999), 15(25), 8627-8632
                          CODEN: LANGD5; ISSN: 0743-7463
PUBLISHER:                American Chemical Society
DOCUMENT TYPE:            Journal
LANGUAGE:                 English
AB   Solubilization of pyrene and steroid hormones into aqueous solns. of
     an associative polymer, poly(ethylene oxide)-b-poly(propylene
     oxide)-b-(poly(ethylene oxide))-g-poly(acrylic acid)
     (Pluronic-PAA), has been studied.  A dramatic increase of
     solubilization is observed upon formation of micelles above the critical
     micellization temperature (cmt).  The equilibrium partition coeffs. of the
     probes between micelles and water (Km/w) above the cmt strongly
     correlate with the probe's octanol/water partition coefficient (Ko/w).
     The Km/w is increased with the ionization degree of the
     poly(acrylic acid) (PAA) segments.  Preferential solubilization of
     the increasingly hydrophobic compds. into the Pluronic-PAA is
     dominated by the entropic effect.  Comparison of the fraction of
     the probe located in the hydrophobic cores of the micellar
     aggregates for pyrene and estradiol illustrates the degree of
     chemical specificity of the Pluronic-PAA micellar aggregates, which
     is due to the hydrophobicity of the probe.
IT   50-27-1, Estriol
     RL: PEP (Physical, engineering or chemical process); PRP
     (Properties); PROC (Process)
        (solubilization by micellar solns. of acrylic-grafted block
        polyoxyalkylenes)
RN   50-27-1  HCAPLUS
CN   Estra-1,3,5(10)-triene-3,16,17-triol, (16α,17β)- (9CI)
     (CA INDEX NAME)

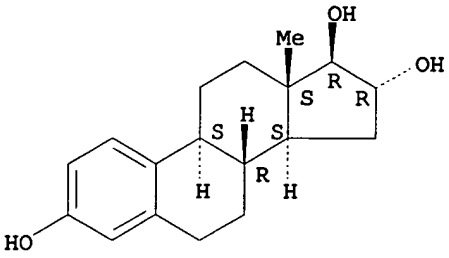
Absolute stereochemistry.
```



CC 37-5 (Plastics Manufacture and Processing)
Section cross-reference(s): **32**, 38, 62, **63**
IT **50-27-1**, Estriol 50-28-2, Estradiol, properties
57-83-0, Progesterone, properties 58-22-0, Testosterone
129-00-0, Pyrene, properties
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(solubilization by micellar solns. of acrylic-grafted block polyoxyalkylenes)
REFERENCE COUNT: 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

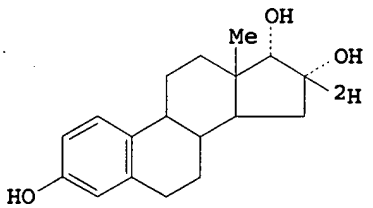
L56 ANSWER 2 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1997:289342 HCAPLUS
DOCUMENT NUMBER: 127:900
TITLE: Influence of the structure of steroid hormones on their association with cyclodextrins: a high-performance liquid chromatography study
AUTHOR(S): Sadlej-Sosnowska, Nina
CORPORATE SOURCE: Drug Institute, Warsaw, 00-725, Pol.
SOURCE: Journal of Inclusion Phenomena and Molecular Recognition in Chemistry (**1997**), 27(1), 31-40
CODEN: JIMCEN; ISSN: 0923-0750
PUBLISHER: Kluwer
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The association consts. of fourteen steroid hormones with β- and γ-cyclodextrin were measured in methanol-water (20:80 volume/volume) at 35 °C using the chromatog. Hummel-Dreyer method. It was found that the greatest influence on the association consts. is the structural features of ring A of these compds. but the substituents of ring D also alter the complex stability to an appreciable degree. The measured association consts. were considerably greater than the corresponding values measured previously in the medium containing more methanol (45 instead of 20%).
IT **50-27-1**, Estriol
RL: PEP (Physical, engineering or chemical process); PROC (Process)
(steroid hormone structure effect on association with cyclodextrins as detected by HPLC)
RN 50-27-1 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16,17-triol, (16α,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 2-2 (Mammalian Hormones)
Section cross-reference(s): **32**, **63**
IT 50-02-2, Dexamethasone 50-24-8, Prednisolone **50-27-1**, Estriol 50-28-2, Estradiol, processes 52-21-1, Prednisolone acetate 53-16-7, Estrone, processes 53-36-1, Methylprednisolone acetate 57-63-6, Ethinylestradiol 68-22-4, Norethisterone 83-43-2, Methylprednisolone 312-93-6, Dexamethasone phosphate 360-63-4, Betamethasone phosphate 378-44-9, Betamethasone 434-22-0, Nandrolone 7585-39-9, β-Cyclodextrin 17465-86-0, γ-Cyclodextrin
RL: PEP (Physical, engineering or chemical process); PROC (Process)
(steroid hormone structure effect on association with cyclodextrins as detected by HPLC)
REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L56 ANSWER 3 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1992:511878 HCAPLUS
DOCUMENT NUMBER: 117:111878
TITLE: NMR studies of estriol
AUTHOR(S): Ling, Yingzhi; Zhang, Zhiliang; Xu, Chunfang; Qiao, Liang
CORPORATE SOURCE: Dep. Pharm. Chem., Beijing Med. Univ., Beijing, Peop. Rep. China
SOURCE: Beijing Yike Daxue Xuebao (**1990**), 22(3), 213-4
CODEN: BYDXEV; ISSN: 1000-1530
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
GI

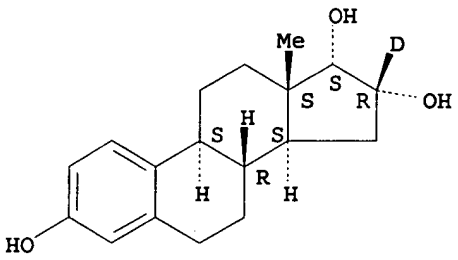


I

AB The carbon-13 NMR spectrum of estriol was reported. Also reported were ATP (attached proton test) and HETCOR spectra of deuterated triol I.
IT **142886-39-3**
RL: PRP (Properties)
(carbon-13 NMR spectra of)
RN 142886-39-3 HCAPLUS
CN Estra-1,3,5(10)-triene-16-d-3,16,17-triol, (16α,17α)-

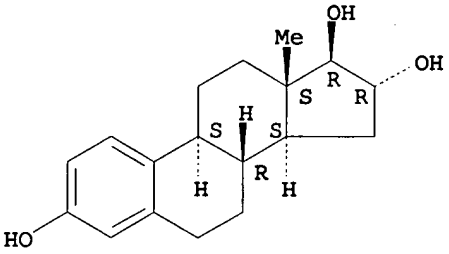
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **50-27-1**, Estriol
RL: PRP (Properties)
(carbon-13 NMR spectrum of)
RN 50-27-1 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16,17-triol, (16α,17β)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



CC 32-3 (**Steroids**)
Section cross-reference(s): **63**, 77
IT **142886-39-3**
RL: PRP (Properties)
(carbon-13 NMR spectra of)
IT **50-27-1**, Estriol 7004-98-0
RL: PRP (Properties)
(carbon-13 NMR spectrum of)

L56 ANSWER 4 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1992:476476 HCAPLUS
DOCUMENT NUMBER: 117:76476
TITLE: Crystallization method for steroids.
INVENTOR(S): Lanquetin, Michel
PATENT ASSIGNEE(S): Laboratoire Theramex S.A., Monaco
SOURCE: PCT Int. Appl., 68 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9208730	A1	19920529	WO 1991-FR888	1991 1112

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W: BR, CA, FI, HU, JP, KR, SU, US
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, NL, SE

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EP 510167	A1	19921028	EP 1992-900237	
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BR 9106012	A	19930105	BR 1991-6012	
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JP 05503305	T2	19930603	JP 1992-500415	
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FI 111545	B1	20030815		
US 5266712	A	19931130	US 1992-910284	
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LV 11183	B	19961020	LV 1995-341	
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PRIORITY APPLN. INFO.:			FR 1990-13981	A
				1990
				1112
			<--	
			WO 1991-FR888	W
				1991
				1112
			<--	

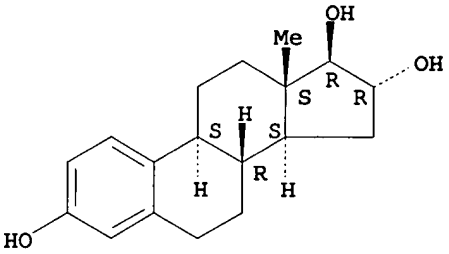
AB A crystallization method is provided whereby a predetd. and homogeneous

particle size class can be obtained nonmech. A substance is dissolved in a ternary mixture consisting of a lipophilic solvent, a hydrophilic solvent and a surface-active agent at a temperature close to boiling. The mixture is allowed to cool to a temperature at which crystallization is initiated and the crystals formed are separated Prednisone was refluxed in a mixture containing Me Et ketone 94.8, water 5.0, and Tween 20 0.2% until dissoln., then cooled at -10° to obtain microcrystals. A tablet contained above crystals 0.5, Avicel PH 102 50.00, Aerosil 1.70, Precirol ATO 5 2.00, and lactose to 130.00 mg.

IT **50-27-1**, Estriol **50-27-1D**, Estriol, ethers and esters
RL: PROC (Process)
(crystallization of, for pharmaceutical formulations)

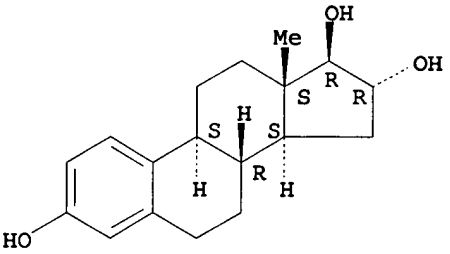
RN 50-27-1 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16,17-triol, (16α,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 50-27-1 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16,17-triol, (16α,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC ICM C07J001-00
ICS A61K031-56; C07J005-00; C07J007-00; C07J011-00

CC 63-5 (**Pharmaceuticals**)
Section cross-reference(s): **32**

IT 50-02-2, Dexamethasone 50-02-2D, Dexamethasone, esters 50-23-7, Hydrocortisone **50-27-1**, Estriol **50-27-1D**, Estriol, ethers and esters 50-28-2, Estradiol, properties 50-28-2D, Estradiol, ethers and esters 53-03-2, Prednisone 53-06-5, Cortisone 53-06-5D, Cortisone, esters 53-16-7, Estrone, properties 53-16-7D, Estrone, ethers and esters 14982-53-7D, Cholestane, derivs. 24749-37-9D, Estrane, derivs. 24887-75-0D, Androstane, derivs. 39219-28-8 58652-20-3, Nomegestrol acetate 58691-88-6, Nomegestrol 58691-88-6D, derivs. 58691-88-6D, Nomegestrol, esters 102734-72-5D, 19-Nor-pregnane, derivs. 123505-24-8 142715-46-6D, Pregn-4-en-21-ol, derivs. 142735-35-1

142761-13-5 142761-13-5D, ethers and esters
RL: PROC (Process)
(crystallization of, for pharmaceutical formulations)

L56 ANSWER 5 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1992:449157 HCAPLUS
DOCUMENT NUMBER: 117:49157
TITLE: Preparation of brain-targeted acyloxymethylphosphonate prodrugs
INVENTOR(S): Bodor, Nicholas S.
PATENT ASSIGNEE(S): USA
SOURCE: PCT Int. Appl., 179 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9200988	A1	19920123	WO 1991-US4824	1991 0712 <--
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US 5177064	A	19930105	US 1990-553548	1990 0713 <--
CA 2087194	AA	19920114	CA 1991-2087194	1991 0712 <--
AU 9183000	A1	19920204	AU 1991-83000	1991 0712 <--
AU 649466	B2	19940526		
EP 539493	A1	19930505	EP 1991-913701	1991 0712 <--
EP 539493	B1	19970326		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
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AT 150759	E	19970415	AT 1991-913701	1991 0712 <--
US 5413996	A	19950509	US 1992-962504	1992 1016 <--
US 5618803	A	19970408	US 1994-340896	1994 1115 <--

PRIORITY APPLN. INFO.: US 1990-553548 A

1990
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WO 1991-US4824 A
1991
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US 1992-962504 A3
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OTHER SOURCE(S): MARPAT 117:49157
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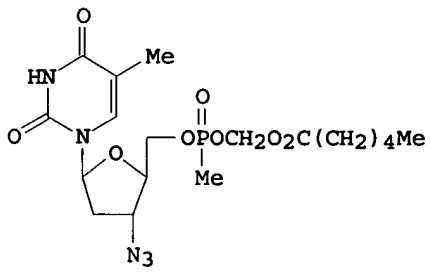


II

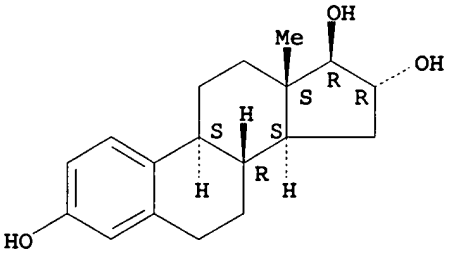
AB QP(O)(R1)OCHR2O2CR3 [Q = O-bonded drug moiety; R1 = alkyl, aryl, aralkyl; R2 = H, hetero)aryl, (cyclo)alkyl, heterocyclyl, aralkyl; R3 = alkyl, alkenyl, (alkyl)cycloalkyl(alkyl), aryloxyalkyl, pyridyl, (substituted) Ph, phenylalkyl], were prepared Thus, zidovudine was stirred with MeP(O)Cl2 and Na2CO3 in acetone for 17 h; H2O was added to give 31.3% zidovudine methylphosphonate (I), which was treated with iodomethyl hexanoate and CsF in DMF to give title compound II. Title compds. are rapidly hydrolyzed in vivo, and I was found in the brain after administration of II.

IT **50-27-1DP**, Estriol, acyloxymethylphosphonate derivative
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as brain-targeted prodrug)

RN 50-27-1 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16,17-triol, (16α,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC ICM C07H019-00
ICS C07J001-00; C07K001-00; A61K031-00; A61K033-00; A61K047-00

CC 33-9 (Carbohydrates)
Section cross-reference(s): **1**, 26, **32**, **63**

IT 50-02-2DP, Dexamethasone, acyloxymethylphosphonate derivative
50-23-7DP, Hydrocortisone, acyloxymethylphosphonate derivative

50-24-8DP, Prednisolone, acyloxymethylphosphonate derivative
50-27-1DP, Estriol, acyloxymethylphosphonate derivative
50-28-2DP, Estradiol, acyloxymethylphosphonate derivative 50-50-0DP,
Estradiol benzoate, acyloxymethylphosphonate derivative 50-89-5DP,
Thymidine, acyloxymethylphosphonate derivative 50-91-9DP,
acyloxymethylphosphonate derivative 52-76-6DP, Lynestrenol,
acyloxymethylphosphonate derivative 53-03-2DP, Prednisone,
acyloxymethylphosphonate derivative 53-06-5DP, Cortisone,
acyloxymethylphosphonate derivative 53-16-7DP, Estrone,
acyloxymethylphosphonate derivative 53-33-8DP, Paramethasone,
acyloxymethylphosphonate derivative 53-34-9DP, Fluprednisolone,
acyloxymethylphosphonate derivative 53-85-0DP,
acyloxymethylphosphonate derivative 54-25-1DP, 6-Azauridine,
acyloxymethylphosphonate derivative 54-42-2DP, Idoxuridine,
acyloxymethylphosphonate derivative 57-63-6DP, Ethinyl estradiol,
acyloxymethylphosphonate derivative 58-18-4DP, Methyl testosterone,
acyloxymethylphosphonate derivative 58-22-0DP, Testosterone,
acyloxymethylphosphonate derivative 58-96-8DP, Uridine,
acyloxymethylphosphonate derivative 61-32-5DP, Methicillin,
silyloxymethylphosphonate derivative 61-33-6DP, Benzylpenicillin,
silyloxymethylphosphonate derivative 61-72-3DP, Cloxacillin,
silyloxymethylphosphonate derivative 66-79-5DP, Oxacillin,
silyloxymethylphosphonate derivative 68-22-4DP, Norethindrone,
acyloxymethylphosphonate derivative 70-00-8DP, Trifluridine,
acyloxymethylphosphonate derivative 72-33-3DP, Mestranol,
acyloxymethylphosphonate derivative 76-25-5DP, Triamcinolone
acetonide, acyloxymethylphosphonate derivative 79-64-1DP,
Dimethisterone, acyloxymethylphosphonate derivative 83-43-2DP,
Methyl prednisolone, acyloxymethylphosphonate derivative 87-08-1DP,
Phenoxymethylpenicillin, silyloxymethylphosphonate derivative
124-94-7DP, Triamcinolone, acyloxymethylphosphonate derivative
127-31-1DP, Fludrocortisone, acyloxymethylphosphonate derivative
147-52-4DP, Nafcillin, silyloxymethylphosphonate derivative
147-94-4DP, Cytarabine, acyloxymethylphosphonate derivative
152-43-2DP, Quinestrol, acyloxymethylphosphonate derivative
152-58-9DP, Cortodoxone, acyloxymethylphosphonate derivative
342-69-8DP, acyloxymethylphosphonate derivative 378-44-9DP,
Betamethasone, acyloxymethylphosphonate derivative 432-60-0DP,
Allylestrenol, acyloxymethylphosphonate derivative 434-03-7DP,
Ethisterone, acyloxymethylphosphonate derivative 605-23-2DP, Ara-T,
acyloxymethylphosphonate derivative 896-71-9DP, Tigestol,
acyloxymethylphosphonate derivative 1035-77-4DP, Estradiol 3-methyl
ether, acyloxymethylphosphonate derivative 1231-93-2DP, Ethynodiol,
acyloxymethylphosphonate derivative 1247-42-3DP, Meprednisone,
acyloxymethylphosphonate derivative 1476-82-0DP,
acyloxymethylphosphonate derivative 1524-88-5DP, Flurandrenolide,
acyloxymethylphosphonate derivative 2135-17-3DP, Flumethasone,
acyloxymethylphosphonate derivative 3056-17-5DP,
acyloxymethylphosphonate derivative 3083-77-0DP,
acyloxymethylphosphonate derivative 3116-76-5DP, Dicloxacillin,
silyloxymethylphosphonate derivative 3124-93-4DP, Ethynerone,
acyloxymethylphosphonate derivative 3511-16-8DP, Hetacillin,
silyloxymethylphosphonate derivative 3643-00-3DP, Oxogestone,
acyloxymethylphosphonate derivative 4097-22-7DP,
acyloxymethylphosphonate derivative 4697-36-3DP, Carbenicillin,
silyloxymethylphosphonate derivative 5536-17-4DP, Vidarabine,
acyloxymethylphosphonate derivative 6533-00-2DP, Norgestrel,
acyloxymethylphosphonate derivative 6736-58-9DP, 3-Deazaadenosine,
acyloxymethylphosphonate derivative 6795-60-4DP, Norvinisterone,
acyloxymethylphosphonate derivative 7481-89-2DP, Dideoxycytidine,
acyloxymethylphosphonate derivative 13563-60-5DP, Norgesterone,
acyloxymethylphosphonate derivative 15176-29-1DP,
acyloxymethylphosphonate derivative 16915-71-2DP, Cingestol,
acyloxymethylphosphonate derivative 18417-89-5DP,
acyloxymethylphosphonate derivative 23205-42-7DP, 3-Deazauridine,
acyloxymethylphosphonate derivative 25526-93-6DP,

acyloxymethylphosphonate derivative 26774-90-3DP, Epicillin,
silyloxymethylphosphonate derivative 26787-78-0DP,
silyloxymethylphosphonate derivative 30516-87-1DP, Zidovudine,
acyloxymethylphosphonate derivative 31698-14-3DP, Cyclocytidine,
acyloxymethylphosphonate derivative 34787-01-4DP, Ticarcillin,
silyloxymethylphosphonate derivative 35943-35-2DP, Triciribine,
acyloxymethylphosphonate derivative 36791-04-5DP, Ribavirin,
acyloxymethylphosphonate derivative 41107-56-6DP,
acyloxymethylphosphonate derivative 53910-25-1DP, Pentostatin,
acyloxymethylphosphonate derivative 54262-83-8DP,
acyloxymethylphosphonate derivative 56039-11-3DP, 3-Deazaguanosine,
acyloxymethylphosphonate derivative 58316-88-4DP,
3-Deazaaristeromycin, acyloxymethylphosphonate derivative
59277-89-3DP, Acyclovir, acyloxymethylphosphonate derivative
60084-10-8DP, Tiazofurin, acyloxymethylphosphonate derivative
69123-90-6DP, FIAC, acyloxymethylphosphonate derivative
69123-98-4DP, FIAU, acyloxymethylphosphonate derivative
69256-17-3DP, acyloxymethylphosphonate derivative 69304-47-8DP,
BVDU, acyloxymethylphosphonate derivative 69655-05-6DP,
Dideoxyinosine, acyloxymethylphosphonate derivative 69979-46-0DP,
Cyclaradine, acyloxymethylphosphonate derivative 72877-50-0DP,
acyloxymethylphosphonate derivative 82410-32-0DP, Ganciclovir,
acyloxymethylphosphonate derivative 83546-42-3DP,
acyloxymethylphosphonate derivative 83705-13-9DP, Selenazofurin,
acyloxymethylphosphonate derivative 84408-37-7DP, 6-Deoxyacyclovir,
acyloxymethylphosphonate derivative 85236-92-6DP,
acyloxymethylphosphonate derivative 86304-28-1DP, Buciclovir,
acyloxymethylphosphonate derivative 90301-59-0DP,
acyloxymethylphosphonate derivative 105784-82-5DP,
acyloxymethylphosphonate derivative 114522-22-4DP,
acyloxymethylphosphonate derivative 119644-22-3DP,
acyloxymethylphosphonate derivative 119770-71-7DP,
acyloxymethylphosphonate derivative 119770-72-8DP,
acyloxymethylphosphonate derivative 142118-61-4P 142118-62-5P
142118-63-6P 142118-64-7P 142118-65-8DP,
acyloxymethylphosphonate derivative 142186-29-6DP,
acyloxymethylphosphonate derivative 142186-30-9DP,
acyloxymethylphosphonate derivative
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as brain-targeted prodrug)

L56 ANSWER 6 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1990:446267 HCAPLUS
DOCUMENT NUMBER: 113:46267
TITLE: Pharmaceutical formulations for parenteral use containing cyclodextrins and dihydropyridine redox systems
INVENTOR(S): Bodor, Nicholas S.
PATENT ASSIGNEE(S): University of Florida, USA
SOURCE: Eur. Pat. Appl., 125 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 335545	A2	19891004	EP 1989-302719	1989 0320
			<--	
EP 335545	A3	19900926		
EP 335545	B1	19930609		
EP 335545	B2	19980923		

R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE
US 4983586 A 19910108 US 1988-174945
1988
0329
<--
EP 327766 A2 19890816 EP 1988-312016
1988
1219
<--
EP 327766 A3 19900926
EP 327766 B1 19980408
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE
AT 90200 E 19930615 AT 1989-302719
1989
0320
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AU 8931762 A1 19890727 AU 1989-31762
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AU 618995 B2 19920116
CA 1336498 A1 19950801 CA 1989-594911
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JP 02009825 A2 19900112 JP 1989-77938
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JP 2643426 B2 19970820
ZA 8902315 A 19901228 ZA 1989-2315
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US 5017566 A 19910521 US 1989-431222
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1103
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US 5024998 A 19910618 US 1989-448655
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PRIORITY APPLN. INFO.: US 1988-174945 A
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EP 1988-312016 A
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US 1987-139755 A2
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CA 1988-585791 A
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IE 1988-3717 A
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IE 1989-810 A
1989
0314
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EP 1989-302719 A
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0320
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US 1989-431222 A2
1989
1103
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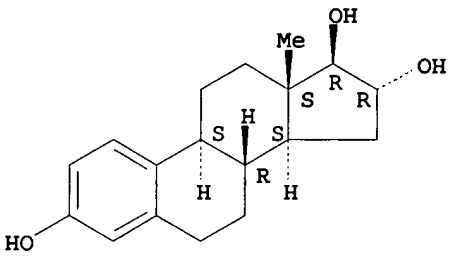
AB Aqueous parenteral solns. of drugs which are insol. or only sparingly soluble and/or which are unstable in water, are combined with a cyclodextrin derivative to provide a means for alleviating problems associated with drug precipitation at the injection site and/or in the lungs or other organs following parenteral administration. Another approach is use of the dihydropyridine-pyridinium redox delivery system. A large number of examples are given for synthesis of dihydropyridine and pyridinium derivs. of drugs. Data are also presented showing drug solubilization by cyclodextrin derivs.

IT **50-27-1**, Estriol
RL: PRP (Properties)
(parenteral delivery systems containing cyclodextrins or pyridine redox systems of)

RN 50-27-1 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16,17-triol, (16α,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC ICM A61K009-08
ICS A61K047-00

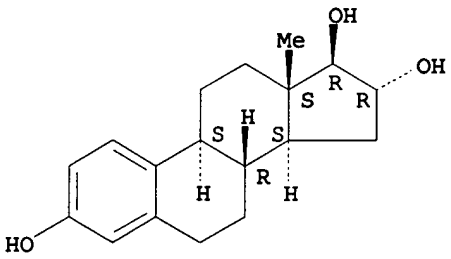
CC 63-5 (**Pharmaceuticals**)
Section cross-reference(s): **1**, 27, 28, **32**, 33

IT 50-02-2, Dexamethasone 50-06-6, Phenobarbital, biological studies 50-23-7, Hydrocortisone 50-24-8 **50-27-1**, Estriol 50-28-2, 17β-Estradiol, biological studies 50-44-2, Mercaptopurine 50-47-5, Desipramine 50-50-0, Estradiol benzoate 51-21-8, 5-Fluorouracil 51-61-6, Dopamine, biological studies 51-98-9 52-01-7, Spironolactone 53-16-7, Estrone, biological studies 53-86-1, Indomethacin 54-31-9, Furosemide 55-63-0, Nitroglycerin 56-12-2, GABA, biological studies 57-41-0, Phenytoin 57-63-6 57-83-0, Progesterone, biological studies 58-00-4, Apomorphine 58-18-4, 17-Methyltestosterone 58-22-0, Testosterone 58-25-3, Chlordiazepoxide 59-05-2, Methotrexate 59-66-5, Acetazolamide 59-92-7, L-DOPA, biological studies 60-18-4, Tyrosine, biological studies 61-32-5, Methicillin 61-33-6, Benzylpenicillin, biological studies 61-54-1, Tryptamine 61-72-3, Cloxacillin 66-76-2, Dicumarol 66-79-5, Oxacillin 67-52-7D, Barbituric acid, derivs. 68-22-4 68-23-5, Norethynodrel 68-26-8, Retinol 69-53-4, Ampicillin 70-00-8, Trifluorothymidine 71-58-9, Medroxyprogesterone acetate 71-63-6, Digitoxin 72-33-3, Mestranol 76-73-3, Secobarbital 76-74-4 77-36-1, Chlorthalidone 99-66-1, Valproic acid 116-31-4, Retinal 127-47-9, Vitamin A acetate 137-58-6, Lidocaine 148-82-3, Melphalan 154-93-8, Car mustine

305-03-3, Chlorambucil 434-03-7 439-14-5, Diazepam 512-64-1, Echinomycin 523-87-5, Dimenhydrinate 604-75-1, Oxazepam 645-05-6, Hexamethylmelamine 745-65-3, Alprostadil 846-49-1, Lorazepam 968-81-0, Acetohexamide 1406-16-2, Vitamin D 1406-18-4, Vitamin E 2365-30-2 2898-12-6, Medazepam 3116-76-5, Dicloxacillin 5104-49-4, Flurbiprofen 6533-00-2, Norgestrel 8064-90-2, Co-trimoxazole 12001-79-5, Vitamin K 12794-10-4D, Benzodiazepine, derivs. 13010-47-4, Lomustine 13182-89-3, Metronidazole benzoate 13909-02-9, PCNU 13909-09-6, Semustine 15676-16-1, Sulpiride 20830-75-5, Digoxin 22204-53-1, Naproxen 22916-47-8 23930-19-0, Alfaxalone 29767-20-2, Teniposide 30516-87-1 31430-15-6, Flubendazole 33125-97-2, Etomidate 33419-42-0, Etoposide 35121-78-9, Prostacyclin 36322-90-4, Piroxicam 41451-75-6, Bruceantin 51264-14-3, Amsacrine 52468-60-7, Flunarizine 57998-68-2, Diaziquone 59277-89-3, Acyclovir 61422-45-5, Carmofur 65277-42-1, Ketoconazole 65886-71-7, Fazarabine 69112-98-7 77327-05-0, Didemnin B 84625-61-6 84697-22-3 127950-65-6
RL: PRP (Properties)
(parenteral delivery systems containing cyclodextrins or pyridine redox systems of)

L56 ANSWER 7 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1987:464732 HCAPLUS
DOCUMENT NUMBER: 107:64732
TITLE: Thermoanalytical study of some steroids. I. Estradiol monovalerate and estriol
AUTHOR(S): De Maury, G.; Masse, J.
CORPORATE SOURCE: Lab. Chim. Gen. Miner., Fac. Pharm., Montpellier, 34060, Fr.
SOURCE: Journal of Thermal Analysis (1986), 31(6), 1263-77
CODEN: JTHEA9; ISSN: 0368-4466
DOCUMENT TYPE: Journal
LANGUAGE: French
AB A thermoanal. study of estradiol monovalerate (I) and estriol (II) showed the thermal stability, the decomposition kinetics, and the temps. and intervals of fusion. The degree of purity was calculated only for I: 99.72 mol %. The fusion enthalpy (29.45 kJ mol-1) and entropy for I were evaluated by DSC. It was also possible to detect the polymorphism and the pseudopolymorphism of I and II after recrystn. from several solvents.
IT **50-27-1**, Estriol
RL: PROC (Process)
(thermal anal. of)
RN 50-27-1 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16,17-triol, (16α,17β)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

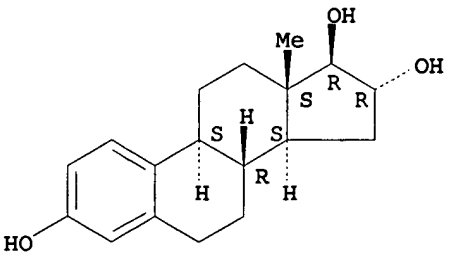


CC 63-5 (**Pharmaceuticals**)
Section cross-reference(s): 22, **32**

IT **50-27-1**, Estriol 27811-56-9, Estradiol monovalerate
RL: PROC (Process)
(thermal anal. of)

L56 ANSWER 8 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1985:46183 HCAPLUS
DOCUMENT NUMBER: 102:46183
TITLE: Diethylsilyl ether and diethylsiliconide derivatives in gas chromatography/mass spectrometry of hydroxylated steroids
AUTHOR(S): Miyazaki, Hiroshi; Ishibashi, Masataka; Itoh, Masahiro; Yamashita, Kouwa
CORPORATE SOURCE: Res. Lab., Nippon Kayaku Co., Tokyo, 115, Japan
SOURCE: Biomedical Mass Spectrometry (**1984**), 11(8), 377-82
CODEN: BMSYAL; ISSN: 0306-042X
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The gas chromatog. and mass spectrometric properties of the diethylsilyl (DEHS) or diethylsiliconide (DES)-DEHS ether derivs. of 20 hydroxysteroids of various types have been studied using N,O-bis(diethylsilyl)trifluoroacetamide as a new silylating agent. The mass spectra of the DES-DEHS ether derivs. were characterized by their marked simplicity and by mol. ions of high abundance, whereas the mass fragmentation patterns of the DEHS ether derivs. without formation of the DES group in the mol. were similar to those of the corresponding dimethylethylsilyl (DMES) ether derivs. The appearance of the mol. ion may be very useful for estimating the mol. weight of hydroxysteroids of which other silyl ether derivs. yield mol. ions of insufficient abundance to characterize them. In particular, the DES-DEHS ether derivative of 5β-pregnane-3α,17α,20α-triol gave the mol. ion at m/z 506 as a principal ion in the electron-impact ionization mode. The methylene unit values of the DEHS ether derivs. of hydroxysteroids without formation of DES groups were slightly larger than those of the corresponding DMES ether derivs. A Δ[Um]s value was presented for estimation of the number of siliconide moieties in the DES-DEHS ether derivs.
IT **50-27-1D**, diethylsilyl ethers and diethylsiliconide derivs. **547-81-9D**, diethylsilyl ethers and diethylsiliconide derivs. **1228-72-4D**, diethylsilyl ethers and diethylsiliconide derivs. **15183-37-6D**, diethylsilyl ethers and diethylsiliconide derivs.
RL: PRP (Properties)
(gas chromatog.-mass spectrum of)
RN 50-27-1 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16,17-triol, (16α,17β)- (9CI) (CA INDEX NAME)

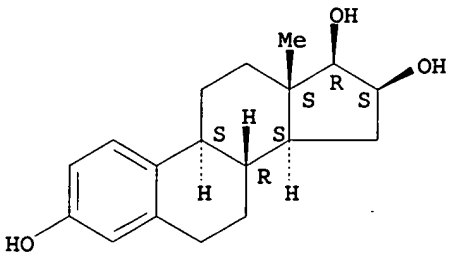
Absolute stereochemistry.



RN 547-81-9 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16,17-triol, (16β,17β)- (9CI)

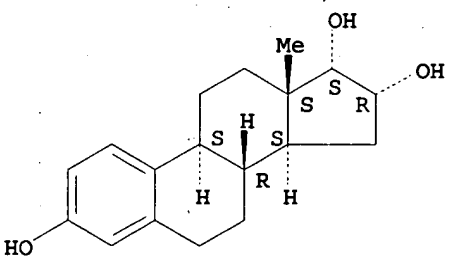
(CA INDEX NAME)

Absolute stereochemistry.



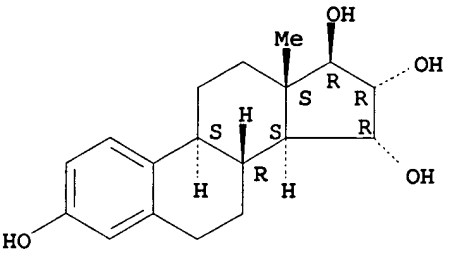
RN 1228-72-4 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16,17-triol, (16α,17α)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



RN 15183-37-6 HCAPLUS
CN Estra-1,3,5(10)-triene-3,15,16,17-tetrol,
(15α,16α,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 32-5 (**Steroids**)
Section cross-reference(s): **64**
IT **50-27-1D**, diethylsilyl ethers and diethylsiliconide
derivs. 50-28-2D, diethylsilyl ethers and diethylsiliconide
derivs. 53-16-7D, diethylsilyl ethers and diethylsiliconide
derivs. 53-43-0D, diethylsilyl ethers and diethylsiliconide
derivs. 58-22-0D, diethylsilyl ethers and diethylsiliconide
derivs. 80-89-7D, diethylsilyl ethers and diethylsiliconide
derivs. 80-92-2D, diethylsilyl ethers and diethylsiliconide
derivs. 80-97-7D, diethylsilyl ethers and diethylsiliconide
derivs. 481-30-1D, diethylsilyl ethers and diethylsiliconide
derivs. 516-53-0D, diethylsilyl ethers and diethylsiliconide
derivs. 516-95-0D, diethylsilyl ethers and diethylsiliconide
derivs. 520-86-5D, diethylsilyl ethers and diethylsiliconide

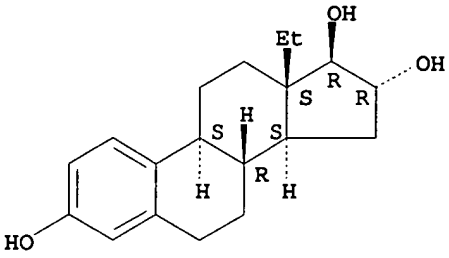
derivs. **547-81-9D**, diethylsilyl ethers and diethylsiliconide derivs. 566-58-5D, diethylsilyl ethers and diethylsiliconide derivs. 570-50-3D, diethylsilyl ethers and diethylsiliconide derivs. 1098-45-9D, diethylsilyl ethers and diethylsiliconide derivs. **1228-72-4D**, diethylsilyl ethers and diethylsiliconide derivs. 1851-23-6D, diethylsilyl ethers and diethylsiliconide derivs. 1852-53-5D, diethylsilyl ethers and diethylsiliconide derivs. **15183-37-6D**, diethylsilyl ethers and diethylsiliconide derivs.
RL: PRP (Properties)
(gas chromatog.-mass spectrum of)

L56 ANSWER 9 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1972:49943 HCAPLUS
DOCUMENT NUMBER: 76:49943
TITLE: Inducing ovulation with compositions comprising 13-alkyl-16α-hydroxy-3,17-dioxygenated-gona-1,3,5(10)-trienes
INVENTOR(S): Edgren, Richard A.
PATENT ASSIGNEE(S): American Home Products Corp.
SOURCE: U.S., 5 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3622670	A	19711123	US 1969-852447	1969 0822
			<--	
PRIORITY APPLN. INFO.:			US 1969-852447 A	1969 0822
			<--	

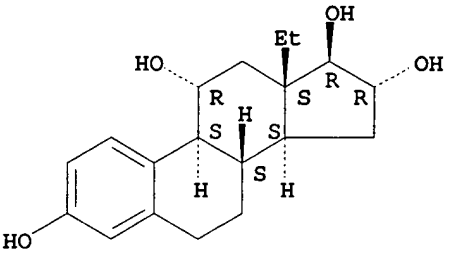
GI For diagram(s), see printed CA Issue.
AB 13-Ethylgona-1,3,5(10)-triene-3,16α,17β-triol (I) and a carrier were used to induce ovulation in warm-blooded anovulatory vertebrates after administration. I was prepared by LiAlH4 reduction of 3,17-diacetoxy-16α,17α-epoxy-1,3,5(10)-triene (II) followed by treatment with EtOAc and 2N HCl. In an example, tablets were prepared from I 5, CM-cellulose 15, lactose 25, redried corn starch 25, Mg stearate 4 mg, and sufficient Ca silicate to give 200 mg of tablet.
IT **19882-03-2 36292-12-3 36292-13-4**
RL: BIOL (Biological study)
(for ovulation induction)
RN 19882-03-2 HCAPLUS
CN Gona-1,3,5(10)-triene-3,16,17-triol, 13-ethyl-, (16α,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



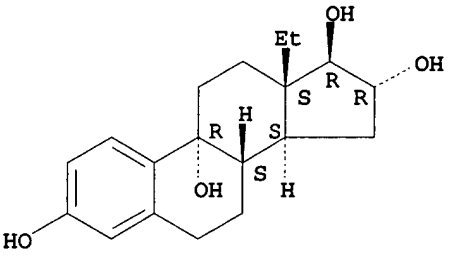
RN 36292-12-3 HCAPLUS
CN Gona-1,3,5(10)-triene-3,11,16,17-tetrol, 13-ethyl-, (11α,16α,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 36292-13-4 HCAPLUS
CN Gona-1,3,5(10)-triene-3,9,16,17-tetrol, 13-ethyl-, (16α,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC A61K
INCL 424238000
CC 63 (**Pharmaceuticals**)
Section cross-reference(s): **32**
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RL: BIOL (Biological study)
(for ovulation induction)

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